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	2025/2026	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 Wei Leyi	Email	zhangqq@mpu.edu.mo
Office	Room N46B, 4/F, Wui Chi Building	Office Phone	85996876

MODULE DESCRIPTION

Chemobioinformatics is an interdisciplinary field that integrates cheminformatics, bioinformatics, and computational drug discovery to accelerate the development of novel therapeutics. This module provides students with cutting-edge computational skills to accelerate drug discovery through cheminformatics, bioinformatics, and artificial intelligence. Participants will learn to leverage pharmaceutical databases, machine learning, and molecular modeling tools (such as RDKit, MOE) and drug design strategies (such as molecular docking, QSAR model, pharmacophore model and AI model) for virtual screening, target prediction, and lead optimization. By integrating cheminformatics (small molecule analysis) with bioinformatics (biological target analysis), students can provide a powerful framework for rational drug discovery and design.

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 computational methods in drug design, including structure-based and ligand-based drug design. (AHEP4-M1, AHEP4-M2)
M2.	Select and apply appropriate chemobioinformatics tools and drug design software, such as MOE, RDkit techniques to perform similarity search, molecular docking, virtual screening, and construct activity prediction and QSAR models. (AHEP4-M3)
M3.	Critically evaluate technical literature and design new computational strategies and be able to use them to solve the practical drug design and discovery problems. (AHEP4-M4, AHEP4-M5)
M4.	Work in a team on an advanced drug discovery research project to design and evaluate a solution to a real-world problem, and finally present it in class. (AHEP4-M16, AHEP4-M17)

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

PILOs	M1	M2	M3	M4
Knowledge and Understanding				
P1. Scientific methodologies and techniques of AI in drug discovery	✓			
P2. Knowledge and in-depth understanding of a wide range of drug discovery-related topics	✓	✓		
P3. Knowledge and hands-on experience of analysis, assessment and solutions of the drug discovery-related issues		✓	✓	
P4. Knowledge and application of AI-related methodologies in innovative solutions				
Skills and Attributes				
P5. Initiate original researches in *in silico* drug discovery, both individually and collaboratively in a team				
P6. Plan, design, execute and manage a scholarly research project				
P7. Critically assess and analyse an advanced technical issue		✓	✓	✓
P8. Communicate research findings, both orally to diverse audiences and in writing through publishing research papers of scholarly values				
P9. Gather and disseminate knowledge at the postgraduate level and beyond	✓			
P10. To demonstrate advanced knowledge, competence and research capability in AI driven drug discovery				
P11. To illustrate a global vision on knowledge advancement and dissemination				
P12. To demonstrate professional integrity and the spirit of challenge			✓	
P13. To advocate professionalism in workplaces and the society at-large				
P14. To communicate professionally and effectively both in speaking and in writing				✓

MODULE SCHEDULE, COVERAGE AND STUDY LOAD

Week	Content Coverage	Contact Hours
1	1. Application of Chemobioinformatics tools in drug discovery and development	3
	1.1 What is Chemobioinformatic?	
	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	2.	Introduction to Pharmaceutical DataBase (PDB)	3
	2.1	KEEG Database	
	2.2	ChemBL Database	
	2.3	Data collection and clean in RDKit	
3-4	3.	Computer representation of chemical molecules	6
	3.1	Computer representations of small molecules (1D, 2D, 3D)	
	3.2	Molecule File Formats	
	3.3	RDkit-Reading, Writing, Manipulating molecules form SMILES	
	3.4	RDkit-Get the atoms and bonds information	
	3.5	RDkit-Molecular Graph representation	
5-7	4.	Molecular Fingerprint and Molecular Similarity	9
	4.1	Molecular Fingerprint	
	4.2	Molecular Similarity	
	4.3	Ligand-based Virtual Screening	
	4.4	RDKit—Molecular Fingerprint Calculation	
	4.5	RDKit—Virtual screening based on molecular similarity	
8-10	5.	ML-based prediction of bioactivity and molecular properties	9
	5.1	Introduction to Biological activity	
	5.2	Introduction to ADMET properties	
	5.3	Molecular filtration based on ADME and Ro5 standards	
	5.4	ML-based prediction of biological activity	
11-13	6.	Introduction to QSAR and Pharmacophore model	9
	6.1	Molecular descriptors	
	6.2	QSAR model building process	
	6.3	Pharmacophore Model construction	
	6.4	MOE-2D-QSAR construction	
	7.	Introduction to drug target and representation	

	7.1	The basic concept of drug target	
	7.2	Receptor as drug target	
	7.3	Enzyme as drug target	
	7.4	Protein structure prediction	
	7.5	PyMOL software introduction	
14-15	8.	Structure-based virtual screening	6
	8.1	Molecular docking	
	8.2	Scoring function	
	8.3	Docking Program	
	8.4	Molecular docking protocol validation	
	8.5	Interactions between drug and target	

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. Coursework/assignment			✓	✓
T3. Group project	✓	✓	✓	✓

ATTENDANCE

Attendance requirements are governed by the Academic Regulations Governing Doctoral 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. Coursework	25	AHEP4-M1, AHEP4-M2,	M1
A2. Assignment	25	AHEP4-M2, AHEP4-M3, AHEP4-M4	M1, M2, M3
A3. Project	50	AHEP4-M4, AHEP4-M5, AHEP4-M16, AHEP4-M17	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/.