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

FACULTY OF APPLIED SCIENCES

MASTER OF SCIENCE IN BIG DATA AND INTERNET OF THINGS

LEARNING MODULE OUTLINE

Academic Year	2024/2025	Semester	2
Module Code	COMP6117		
Learning Module	Selected Topics II: Theory and Practice in Artificial Intelligence driven Drug Discovery		
Pre-requisite(s)	Nil		
Medium of Instruction	English		
Credits	3	Contact Hours	45 hrs
Instructor	Qianqian Zhang Shu Li	Email	zhangqq@mpu.edu.mo shuli@mpu.edu.mo
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MODULE DESCRIPTION

Over the past few years, computer-aided drug design technology and artificial intelligence drug design has played an important role in new drug development. Artificial intelligence can potentially save time and money as well as increase the success rate of new drug development. This module covers the advanced topics of artificial intelligence in drug discovery from target structure prediction, lead discovery to lead optimization and drug-likeness evaluation. The main topics include the basic principles of modern drug discovery, the prediction of drug-target interaction, virtual screening of small molecular database, in silico prediction of properties of drug molecules, de novo drug design. In addition, a brief introduction to conventional methods used in state-of-the-art commercial and non-commercial packages will be provided. This will assist students in better understanding the workflow of the corresponding tools and, at the same time, enhance their capabilities in data analysis.

MODULE INTENDED LEARNING OUTCOMES (ILOS)

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

M1.	Apply the theoretical knowledge of computer aided drug design and artificial intelligence drug design to solve drug discovery and development problems. (AHEP4-M1)
M2.	Apply machine learning, molecular docking, similarity search, pharmacophore model and QSAR model methods to screen the “hit compound” from large chemical databases step-by-step. (AHEP4-M2, AHEP4-M3)
M3.	Critically evaluate and select proper machine learning strategies and be able to use them to solve the practical drug design and discovery problems. (AHEP4-M4)
M4.	Work in a team for a complete an advanced drug discovery research topic, design and evaluate AI solutions for a real-world problem, and finally present it in module. (AHEP4-M5, AHEP4-M7, 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.	Master the principles of system engineering and relevant enabling technologies for building of IoT solutions	✓			
P2.	Critically evaluate scientific methodologies and mathematical models for Big Data and its applications		✓		
P3.	Master the advanced software and programming tools and techniques for IoT solutions and Big Data		✓		
P4.	Explain the processes involved in IoT solutions and Big Data analytics in a typical business setting				
P5.	Explain different application domains and analyze their requirements for IoT and Big Data				
P6.	Apply knowledge in advanced communication and multimedia technologies for the design and implementation of IoT solutions				
P7.	Apply knowledge in applied statistics, machine learning, leading-edge technologies and programming techniques for Big Data			✓	
P8.	Design and carry out an advanced project following an ethical and professional methodology				✓
P9.	To demonstrate advanced knowledge and R&D techniques in Big Data and IoT				
P10.	To investigate and develop new, emerging ICT technology for Big Data and IoT				
P11.	To develop a global vision on the critical development and new application of Big Data and IoT				✓
P12.	To communicate technically and effectively in both speaking and writing				✓
P13.	To have a positive attitude towards society and the environment.				
P14.	To adhere to high moral standards and commit to excellence in life-long learning.				✓

MODULE SCHEDULE, COVERAGE AND STUDY LOAD

Week	Content Coverage	Contact Hours
1	1. Introduction to drug discovery and development	3
	1.1 What are drugs?	

	1.2	What are proteins and drug targets?	
	1.3	The discovery and development process of drugs	
	1.4	Introduction to computer-aided drug design (CADD)	
	1.5	Introduction to artificial intelligence drug design (AIDD)	
2-3	2.	Introduction to drug target types and representations	6
	2.1	The basic concept of drug target	
	2.2	Receptor as drug target	
	2.2	Enzyme as drug target	
	2.2	Protein structure and function	
	2.2	PyMOL software introduction	
4-5	2.	Structure-based drug discovery	6
	2.1	Molecular docking	
	2.2	Scoring function	
	2.3	Docking Program	
6-7	3.	Ligand-based drug discovery	6
	3.1	Conformational Sampling of Ligand	
	3.2	Fingerprint/Descriptors-based search	
	3.3	Pharmacophore model	
	3.4	Quantitative structure–activity relationships (QSAR) model	
8-9	4.	AI-based Drug-target Binding Prediction	6
	4.1	Binding site prediction	
	4.2	Searching the conformational space for docking	
	4.3	Machine learning-based scoring functions	
	4.4	Benchmarking dataset	
10-12	5.	Database in AIDD research	9
	5.1	Target Database	
	5.2	Molecular Database	
	5.3	Peptide Database	
	5.4	Antibody Database	

13-15	6.	AI enhanced Molecular Dynamics Simulations	9
	6.1	MD simulation history	
	6.2	MD simulation process	
	6.3	Force Field	
	6.4	MD simulation software	

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 Master'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. Assignment	25%	AHEP4-M1, AHEP4-M2, AHEP4-M3, AHEP4-M4	M1, M2, M3
A2. Test	25%	AHEP4-M1, AHEP4-M2, AHEP4-M3, AHEP4-M4,	M1, M2, M3
A3. Project	50%	AHEP4-M5, AHEP4-M7, 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.

Students with an overall score of less than 35 in the coursework will fail the module even if the overall score for the module is 50 or above.

Students with a score of less than 35 in the final examination will fail the module even if the overall score for the module is 50 or above.

REQUIRED READINGS

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

REFERENCES

1. Gisbert Schneider (2014). *De novo* Molecular Design, Wiley-VCH.
2. Nathan Brown (2021). Artificial Intelligence in Drug Discovery, Royal Society of Chemistry.
3. Alexander Heifetz (2022). Artificial Intelligence in Drug Design, Humana Press.

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/.