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	AIDD8122		
Learning Module	Advanced Topics in Artificial Intelligence & Drug Discovery		
Pre-requisite(s)	Nil		
Medium of Instruction	Chinese and English		
Credits	3	Contact Hours	45 hrs
Instructor	XiaoJun Yao Zhuyifan Ye Shu Li (Contact person)	Email	shuli@mpu.edu.mo
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MODULE DESCRIPTION

This module explores the transformative role of artificial intelligence (AI) in modern drug discovery, equipping students with the theoretical foundations, advanced methodologies, and practical skills necessary to utilize AI in solving complex problems in the pharmaceutical field. Students will gain comprehensive knowledge of AI techniques, including machine learning, deep neural networks, attention mechanisms, and transformer architectures, and their applications in areas such as molecular docking, biomolecular structure prediction, and de novo drug design. Students will engage in critical evaluation of AI strategies, develop innovative solutions to address drug discovery challenges, and analyze emerging trends and future directions in the field.

MODULE INTENDED LEARNING OUTCOMES (ILOS)

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

M1.	Understand the theoretical and practical foundations of AI and its transformative role in drug discovery, including basic principles of machine learning and its applications in the pharmaceutical field. (AHEP4-M1)
M2.	Apply advanced AI methods, including neural networks (deep and recurrent), attention mechanisms, and transformer models, to solve specific computational methods. (AHEP4-M3)
M3.	Critically evaluate and compare diverse AI strategies for drug discovery, including de novo design, molecular docking, and biomolecular structure prediction, to plan effective computational workflows. (AHEP4-M2, AHEP4-M4)
M4.	Undertake a comprehensive project to design and implement AI-driven solutions for real-world drug discovery problems, including hands-on practice, evaluation of outcomes, and effective communication of results through scientific presentations. (AHEP4-M5, AHEP4-M17)
M5.	Analyze emerging challenges in AI-driven drug discovery, such as molecular structure prediction and molecular dynamics simulation, and propose future research directions to address unresolved scientific and computational issues. (AHEP4-M2)

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

PILOs	M1	M2	M3	M4	M5
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	Applications of AI in Drug Discovery: Opportunities and Challenges	3
2	Introduction to Machine Learning, Learning Algorithms, Hypothesis Function, Loss Function, and Various Machine Learning Algorithms	3
3	Neural Network, Back Propagation, and Gradient Decent Optimization Algorithms	3
4	Deep Neural Network, Convolutional Neural Networks, Training technologies, Recurrent Neural Networks, LSTM, Encoder-Decoder Architecture, and Transformers	3

5	Lab practice 1	3
6	AI in *de novo* Drug Design	3
7	AI Drug Discovery Database	3
8	AI in Biomolecular Structure Prediction	3
9	AI-based Molecular Docking	3
10	Combined AI and Molecular Dynamics Simulation	3
11	Lab practice 2	3
12	Individual student presentation 1	3
13	Individual student presentation 2	3
14	Individual student presentation 3	3
15	Individual student presentation 4	3

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**	**M5**
T1. Lectures	✓	✓	✓		✓
T2. Lab practice		✓	✓	✓	✓
T3. Assignments, projects and student presentations	✓	✓	✓	✓	✓

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. Assignment A (by Dr. Ye)	15%	AHEP4-M1, AHEP4-M3	M1, M2
A2. Assignment B (by Dr. Li)	15%	AHEP4-M1, AHEP4-M2, AHEP4-M4	M1, M3, M5
A3. Final Project (individual student report and presentation)	70%	AHEP4-M1, AHEP4-M2,	M1, M2, M3, M4, M5

		AHEP4-M3, AHEP4-M4, AHEP4-M5, AHEP4-M17	

This learning module is graded on a 100 point scale, with 100 being the highest possible score and 50 being the passing score. There is no final examination, no re-sit examination and no supplementary examination in this module.

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.

REQUIRED READINGS

As specified during the module: scientific literature and journal articles.

REFERENCES

Reference book(s)

1. Shai Shalev-Shwartz and Shai Ben-David (2014). *Understanding Machine Learning: From Theory to Algorithms.* Cambridge University Press.
2. Ian Goodfellow, Yoshua Bengio and Aaron Courville (2016). *Deep Learning.* An MIT Press book, http://www.deeplearningbook.org.
3. Alexander Heifetz (2022). Artificial Intelligence in Drug Design (Methods in Molecular Biology, 2390) 1st ed.

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/.