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	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

Artificial Intelligence (AI) is so pervasive today that possibly you are using it in one way or the other and you don't even know about it. Deep learning is the embodiment of AI in the current era. In the past decade, deep learning has given us many amazing applications such as computer vision, natural language processing, AlphaFold, large language models etc. This module covers some of the most important methods for AI, such as machine learning, deep neural networks, attention mechanism, etc. This module also explains how to apply AI techniques in drug discovery and development, including protein structure prediction, virtual screening, and AI-assisted molecular dynamics (MD) simulations. The aim of the module is to give students the important trends of AI techniques, and to allow them to apply such methods in drug discovery and development by practice.

MODULE INTENDED LEARNING OUTCOMES (ILOS)

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

M1.	Apply the artificial intelligence knowledge and mathematics to solve drug discovery related problems.
M2.	Critically evaluate and select proper machine learning strategies and be able to use them to perform drug discovery related computational tasks.
M3.	Work in a team for a complete drug discovery related project, design and evaluate machine learning solutions for a real-world problem, and finally present it in class.
M4.	Understand the principles and significance of AI in protein structure predictions, virtual screening and MD.
M5.	Discuss the current challenges and future directions of AI in drug design and development.

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

PILOs	M1	M2	M3	M4	M5
P1. To demonstrate understanding in scientific methodologies and techniques of AI in drug discovery	✓			✓	✓
P2. To demonstrate of knowledge and in-depth understanding of a wide range of AI drug discovery related topics	✓			✓	✓
P3. To demonstrate knowledge and hands-on experience of analysis, assessment and solutions of the AI drug discovery related issues		✓	✓	✓	✓
P4. To apply professional knowledge of AI-related methodologies in innovative solutions		✓	✓	✓	✓
P5. To initiate original researches in *in-silico* drug discovery, both individually and collaboratively in a team		✓	✓	✓	
P6. To plan, design, execute and manage a scholarly research project		✓	✓	✓	
P7. To critically assess and analyse an advanced technical issue		✓	✓		✓
P8. To communicate research findings, both orally to diverse audiences and in writing through publishing research papers of scholarly values.			✓		
P9. To gather and disseminate knowledge at the postgraduate level and beyond	✓	✓	✓		✓
P10. To demonstrate professional ethics & integrity, and the spirit of challenge			✓		✓

MODULE SCHEDULE, COVERAGE AND STUDY LOAD

Week	Content Coverage	Contact Hours
1	1. Applications of Artificial Intelligence in Drug Discovery: Opportunities and Challenges	3
2	2. Introduction to Machine Learning, Learning Algorithms, Hypothesis Function, Loss Function, and Various Machine Learning Algorithms	3
3	3. Neural Network, Back Propagation, and Gradient Decent Optimization Algorithms	3
4	4. Deep Neural Network, Convolutional Neural Networks, and Training technologies	3
5	5. Recurrent Neural Networks, LSTM, Encoder-Decoder Architecture, and Transformers	3
6	6. Lab practice I	3
7	7. Artificial intelligence in *de novo* drug design	3
8	8. AI & ML Drug Discovery Database	3
9	9. AI in Biomolecular Structure Predictions	3
10	10. AI-based Molecular Docking	3
11	11. Combined AI and Molecular Dynamics Simulation	3
12	12. Lab practice II	3

13	13. Individual student presentation I	3
14	14. Individual student presentation II	3
15	15. Individual student presentation III	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. 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 (%)	ILOs to be Assessed
A1. Assignment A (by Dr. Ye)	15%	M1, M2
A2. Assignment B (by Dr. Li)	15%	M1, M4, M5
A3. Individual student report	40%	M3
A4. Individual student presentation	30%	M3

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/.