



FACULTY OF APPLIED SCIENCES
DOCTOR OF PHILOSOPHY IN ARTIFICIAL INTELLIGENCE DRIVEN DRUG DISCOVERY
LEARNING MODULE OUTLINE

Academic Year	2025/2026	Semester	1
Module Code	AIDD8123		
Learning Module	Frontiers in Drug Discovery and Development		
Pre-requisite(s)	None		
Medium of Instruction	Chinese and English		
Credits	3	Contact Hours	45
Instructor	Dr. Duan Hong Liang (Contact person) Dr. Tong Hoi Yee, Henry	Email	hduan@mpu.edu.mo
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MODULE DESCRIPTION

Societies across the world are looking to combat a greater range of human diseases but at the same time contain spiralling healthcare costs. This, together with global competition and increasing regulatory standards, puts enormous pressure on the pharmaceutical industry to discover and develop a greater number of therapeutic candidates even faster and cheaper than ever before. This module develops the key themes in the drug discovery and development pipeline and highlights the multi-disciplinary nature of the research and development process. The module deals with different phases in drug development, including target identification and validation, hit discovery, hit-to-lead optimization, pre-clinical and clinical testing, registration and commercialisation, regulatory and manufacturing considerations.

MODULE INTENDED LEARNING OUTCOMES (ILOS)

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

M1.	Analyze how different fields (like computational chemistry and AI) work together in drug discovery stages (AHEP4-M1)
M2.	Evaluate decision-making science and risks in drug development (AHEP4-M2)
M3.	Use AI models to solve drug development problems and communicate, and explain these methods for drug studies. (AHEP4-M3, AHEP4-M5, AHEP4-M17)
M4.	Combine research, patent, and business data for drug intelligence (AHEP4-M4)
M5.	To evaluate scientific, ethical and market-related considerations of importance in the drug development (AHEP4-M7)

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

PILOs	M1	M2	M3	M4	M6
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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 <i>in silico</i> 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	Basic concepts in drug discovery and development (Dr. Tong)	3
2	Overview in pharmaceutical industry (Dr. Tong)	3
3	Structure-based lead compound discovery (Dr. Duan)	3
4	Deep Learning in lead compound optimization (Dr. Duan)	3
5	Lead compound optimization based on drug metabolism and pharmacokinetics (Dr. Duan)	3
6	Pharmacokinetics in drug discovery and development (Dr. Duan)	3
7	Machine Learning for In Silico ADMET Prediction (Dr. Duan)	3
8	Lead compound optimization based on improving drug efficacy (Dr. Duan)	3
9	Chemical synthesis for small molecules (Dr. Duan)	3
10	Deep Learning in drug synthesis (Dr. Duan)	3



11	Student presentation A (Dr. Duan)	3
12	Artificial intelligence in Protein/Peptide Structure Prediction (Dr. Duan)	3
13	Clinical trial in drug discovery and development (Dr. Duan)	3
14	Due diligence for biotechnology and pharmaceutical companies (Dr. Duan)	3
15	Student presentation B (Dr. Duan)	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	M6
T1. Lectures	✓	✓	✓	✓		
T2. Course works	✓	✓	✓	✓	✓	✓
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 (%)	AHEP4 LOs	ILOs to be Assessed
A1. Course work A (by Dr. Duan)	50%	AHEP4-M2, AHEP4-M4, AHEP4-M7	M2, M4, M5
A2. Individual student presentation A (by Dr. Duan)	25%	AHEP4-M1, AHEP4-M3, AHEP4-M5, AHEP4-M17	M1, M3
A3. Individual student presentation B (by Dr. Duan)	25%	AHEP4-M1, AHEP4-M3, AHEP4-M5, AHEP4-M17	M1, 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



Module resources as provided including copies of PowerPoint slides, as well as additional reading/recommended texts.

Weblinks: as specified during the module; scientific literature and journal articles.

REFERENCES

Benjamin Blass. (2021) Basic Principles of Drug Discovery and Development (2nd edition). Elsevier, London, U.K.

Raymond G Hill, Duncan Richards. (2021) Drug Discovery and Development Technology in Transition (3rd edition). Elsevier, London, U.K.

Alexander Heifetz. (2022) Artificial Intelligence in Drug Design. Springer.

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/.