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

FACULTY OF APPLIED SCIENCES

BACHELOR OF SCIENCE IN COMPUTING

LEARNING MODULE OUTLINE

Academic Year	2023/2024	Semester	2
Module Code	COMP409		
Learning Module	Selected Topics IV - Introduction to Artificial Intelligence driven Drug Discovery		
Pre-requisite(s)	Nil		
Medium of Instruction	English		
Credits	3	Contact Hours	45 hrs
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MODULE DESCRIPTION

Computer-aided drug design (CADD) and artificial intelligence driven drug design (AIDD) has played important role in new drug discovery and development. CADD and AIDD can potentially save time and money as well as increase the success rate of new drug development. This module covers the basic theories and concepts of CADD and AIDD, as well as their applications in different stages of drug discovery. The main topics include the virtual screening, drug-target interaction prediction, protein structure prediction, pharmacophore model, de novo molecular generation et al. During the study, students will have the basic understand of drug discovery and computer-aided, AI-based 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.	Understand the basic theories and concepts of computer-aided drug design and artificial intelligence driven drug design. (*SM1p, SM2p*)
M2.	Apply critical thinking skills to identify research problems, evaluate potential solutions, and make informed decisions in the drug design process. (*D2p*)
M3.	Apply computational tools and software for drug design, such as molecular docking, virtual screening, and molecular dynamics simulations.; (*EA3p, EA4p*)
M4.	Develop a mindset of continuous learning, staying updated with the latest advancements in the field of drug design and related technologies. (*EP7p, ET4p*)

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

PILOs		M1	M2	M3	M4
P1.	Select and apply proven methods, tools and techniques to the effective and efficient implementation of information systems;		✓		
P2.	Evaluate computer systems in a local area network, and understand the additional requirements for connection to other networks through wide area networks;				✓
P3.	Be competent in system development in the Internet and the web platform;				
P4.	Work independently to design and implement a relational database, with an emphasis on how to organise, maintain and retrieve information from a DBMS;		✓	✓	
P5.	Acquire essential knowledge in specific fields of computing disciplines including multimedia, security and artificial intelligence;	✓			✓
P6.	Acquire the perceptive skills needed to understand information presented in the form of UML diagram, flow chart or other industry standard formats;				
P7.	Understand the need for and use of the necessary mathematical techniques;		✓		✓
P8.	Work independently to develop an understanding of, and the knowledge and skills associated with the general support of computer systems and networks;			✓	
P9.	Work as an effective member of a team in the analysis, design and development of software systems;				
P10.	Use project planning and management techniques in systems development;				
P11.	Understand the fundamental and operational issues of computer systems in business environments;		✓		
P12.	Equip with adequate written, oral communication and interpersonal skills;				
P13.	Build the capacity and desire for lifelong learning and to learn advanced and emerging technologies on one's own;				✓
P14.	(For Enterprise Information Systems specialization) Gain an in-depth understanding of the information technology related to enterprise information systems, with an emphasis on development of such systems to support business processes;				
P15.	(For Gaming Technology specialization) Acquire the general and advanced knowledge of current technologies and operating environment in the gaming industry;				
P16.	(For Computer Education specialization) Acquire the general and practical knowledge of computer education and its practicing environment in secondary education.				

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	Draw small molecule structures	
	1.5	Molecular descriptors	
	1.6	Molecular Fingerprint	
2-3	2.	Structure-based drug discovery	6
	2.1	Molecular docking	
	2.2	Scoring function	
	2.3	Docking Program	
	2.4	De novo drug design	
4-5	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	
6	4.	Density functional theory and its applications in drug discovery	3
	4.1	Wave-function-based and charge-density-based methods	
	4.2	Hartree-Fock approximation and Kohn-Sham equation	
	4.3	Density functional theory basis sets	
	4.4	Applications	
7-10	5.	Introduction to Computational Methods	12
	5.1	Basic mathematical operations	
	5.2	Ordinary differential equation	
	5.3	2nd order differential equation	
	5.4	Classic Monte Carlo methods	

11-15	6.	How Artificial Intelligence is Revolutionizing Drug Discovery	15
	6.1	Drug discovery database applications	
	6.2	Biomolecular structure predictions	
	6.3	Artificial intelligence-based Virtual Screening	
	6.4	Combined Artificial Intelligence and molecular dynamic methods	

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 Bachelor'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 (%)	AHEP3 LOs	ILOs to be Assessed
A1. Assignment	25 %	*D2p, EA3p, EA4p*	M2, M3
A2. Test	25 %	*SM1p, SM2p, EP7p, ET4p*	M1, M2, M4
A3. Examination	50 %	*SM1p, SM2p, EP7p, ET4p*	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 must take the re-sit examination even if the overall score for the module is 50 or above.

Students with a score of less than 35 in the final examination must take the re-sit examination even if the overall score for the module is 50 or above.

Students with an overall final grade of less than 35 are NOT allowed to take the re-sit examination.

REQUIRED READINGS

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

REFERENCES

1. Nathan Brown (2021). Artificial Intelligence in Drug Discovery, Royal Society of Chemistry.
2. Alexander Heifetz (2022). Artificial Intelligence in Drug Design, Humana Press.
3. Martin, R.M. (2020). Electronic structure: basic theory and practical methods. Cambridge University 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/.