Jordan University of Science and Technology
Faculty of Pharmacy
Pharmacy Department

PHAR781 Molecular Modeling And Computer-Aided Drug Design

First Semester 2024-2025

Course Catalog
3 Credit Hours. This course covers the theory of molecular modeling, including force fields, energy minimization, molecular dynamics, homology modelling and their applications in drug design. In addition, it covers theory and practice of most currently used computational techniques in the field of computer-aided drug design, including approaches for both ligand and target drug design such as similarity searching, pharmacophore modeling, QSAR, structure-based drug design (docking and scoring), virtual screening, and ADMET property prediction.
Teaching Method: Blended

Text Book	
Title	Molecular Modelling: Principles and Applications
Author(s)	Andrew Leach
Edition	2nd Edition
Short Name	ref #1
Other Information	

Course References

Short name	Book name	Author(s)	Edition	Other Information
Ref #2	Drug Design Structure and Ligand-Based Approaches	Kenneth M. Merz, Dagmar Ringe Charles H. Reynolds	3rd Edition	

Instructor	
Name	**Dr. RUFAIDA AL ZOUBI**
Office Location	P2 - L-2 room 106
Office Hours	
Email	rmalzoubi1@just.edu.jo

Class Schedule & Room
Section 2: Lecture Time: Tue : 08:30 - 10:30 Room: قاعة الندوات/صيدلة

Tentative List of Topics Covered

Weeks	Topic	References
Week 1	Introduction to computational drug design	From **ref #1**
Week 2	Revision of protein structure and intermolecular and intramolecular interactions	From **Ref #2**
Week 3	Graphical representations, molecular coordinates, and small molecule notations	From **ref #1**
Week 4	Molecular conformation, energy minimization, quantum mechanical energy and molecular mechanics forcefields.	From **ref #1**
Week 5	Ligand docking and virtual screening	From **ref #1**
Week 6	Pharmacophore modelling	From **ref #1**
Week 7	QSAR, ADMET and molecular descriptors	From **ref #1**
Weeks 8, 9	Molecular dynamics simulations, theory and application	From **ref #1**, From **Ref #2**
Weeks 10, 11, 12, 13, 14, 15, 16	Project and seminar	

Mapping of Course Outcomes to Program Outcomes	Course Outcome Weight (Out of 100%)	Assessment method
Explain quantum mechanics and molecular mechanics forcefields and their applications in drug design. [20PLO-MP1]	20%	First exam (Theoretical), Final project defense and presentation
Use websites and modeling software relevant to computer-aided drug discovery and design. [25PLO-MP2]	25%	Hands-on lab work, Final project defense and presentation

Evaluate drug-protein interactions based on a knowledge of intermolecular interactions and conformational energy profiles. [25PLO-MP2]	25%	First exam (Theoretical), Final project defense and presentation
Apply different computational techniques such as ligand and protein preparation and minimization, docking, and pharmacophore modeling in drug design. [30PLO-MP3]	30%	Hands-on lab work, Final project defense and presentation

PLO1.1	PLO2.1	PLO3.2	PLO3.3	PLO2.2	PLO2.3	PLO2.4	PLO3.1	PLO3.4	PLO3.5	PLO3.6	PLO4.1	PLO4.2	PLO4.3	PLO4.4	PLO5.1	PLO-PT1.1	PLO-PT2.1	PLO-PT2.2	PLO-PT3.1

Evaluation	
Assessment Tool	**Weight**
First exam (Theoretical)	25%
Hands-on lab work	25%
Final project defense and presentation	50%

Date Printed: 2024-10-09