Detailed Course Description - Course Plan Development and Updating Procedures/ Pharmacy Department	QF02/0408-3.0E

Faculty	Pharmacy	Department	Pharmacy
Course number	**201742**	Course title	**Advanced Medicinal Chemistry and Drug Design**
Number of credit hours	3	Pre-requisite/co-requisite	

Brief course description

This course is designed to impart the knowledge in computational methods and drug design approaches. It aims to build students' knowledge in theoretical chemistry and its application in drug design. It is proposed to provide students with an understanding of hit discovery, lead identification, lead optimization, target selection, and molecular recognition employing computer-aided drug design software. And, it will shed the light on computer-based methods, combinatorial chemistry, high-throughput screening, and database mining.

	Course goals and learning outcomes
Goal 1	To distinguish between bioinformatics and cheminformatics methods and their recruitment in drug design.
Learning outcomes	1.1 Recognize theoretical strategies and their classifications. 1.2 Describe the drug design pipeline and understand where computational chemistry fits in. 1.3 Discuss informatics approaches to the prediction of chemical properties. 1.4 Understand the importance of drug-like properties and their prediction. 1.5 Describe the use of lead candidates and database representations. 1.6 Understand the use of classifier algorithms and quantum/classical descriptors. 1.7 Describe relations between thermodynamic properties and protein-ligand binding and structure. 1.8 Describe protein-ligand docking and the empirical/knowledge-based scoring functions. 1.9 Discuss empirical scoring, de-novo design and virtual screening. 1.10 Describe simulations of ligand binding thermodynamics. 1.11 Appreciate protein sequence searches, homology and loop modelling, protein-protein docking, and describe biologics design. 1.12 Describe the relation between IC_{50} and Kd, and discuss biophysical methods. 1.13 Know how to use software such as MOE, MAESTRO, AMBER, and PYMOL.
Textbook	1. The Organic Chemistry of Drug Design and Drug Action, 2nd edition, Richard B. Silverman, Elsevier, 2004. 2. Foye's Principles of Medicinal Chemistry, 6th edition, Thomas L. Lemke and David A. Williams, Lippincott Williams & Wilkins, 2008.

	3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th edition, J. N. Delgado and W. A. Remers, Lippincott-Raven, 2011. 4. Burger's Medicinal Chemistry and Drug Discovery, 6th edition, M. E. Wolff, 2003.
Supplementary references	1- An Introduction of Medicinal Chemistry, 4th edition, Graham Patrick, Oxford University Press, 2008. 2- The Organic Chemistry of Drug Synthesis, Vol. 1-6, D. Lednicer and L. A. Mitscher, John Wiley and Sons. 3- Computational Chemistry and Drug design Journals.

Course timeline				
Week	**Number of hours**	**Course topics**	**Pages (textbook)**	**Notes**
01	**1** **1** **1**	- Computational Methods - Potential energy. - Molecular mechanics. - Quantum Mechanics. - Geometry Optimization. - First Order Minimization. - Second Order Minimization.	Textbooks 1-3/ Drug Design Part	
02	**1** **1** **1**	- Conformational Analysis. - Molecular Dynamic (MD) Simulation. - Monte Carlo Method. - Metropolis Method. - NPT Model - NVT Model.	Textbooks 1-3/ Drug Design Part	
03-04	**2** **2** **2**	- X-ray crystallography - Homology Modeling - Bioinformatics. - Structure-Based Drug Design - Molecular Docking - Binding Free Energy.	Textbooks 1-3/ Drug Design Part	

05-06	**2 2 2**	- Ligand-Based Drug Design. - Cheminformatics. - Pharmacophore Modeling - Pharmacophore Searching - Druggability - Lipinski's Rule of Five - Database Mining - Virtual Screening	Textbooks 1-3/ Drug Design Part	
07-08	**2 2 2**	- Ligand-Based Drug Design - Quantitative Structure-Activity Relationship - Equations and Graphs. - Physicochemical Properties. - Hydrophobicity. - Electronic Property. - Steric Factor. - Craig Plot. - Topliss Scheme. - Hansch Equation. - Topliss operational schemes. - QSAR: 3D-QSAR (CoMFA).	Textbooks 1-3/ Drug Design Part	
09	**1 1 1**	- Combinatorial Chemistry. - Parallel Synthesis. - Solid Phase Technique. - High-Throughput Screening.	Textbooks 1-3/ Drug Design Part	
10	**1 1 1**	- Case Study I	Textbooks 1-3/ Drug Design Part	
11	**1 1 1**	- Case Study II	Textbooks 1-3/ Drug Design Part	
12	**1 1 1**	Article Presentation and Discussion.	Computational Chemistry and Drug design Journals.	
13	**1 1 1**	Molecular Modeling Practical	Modeling Lab Applications	

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Theoretical course evaluation methods and weight	Participation = 10% First exam 20% Second exam 20% Final exam 50%	**Practical (clinical) course evaluation methods**	Semester students' work = 50% (Reports, research, quizzes, etc.) Final exam = 50%

Approved by head of department		**Date of approval**	

Extra information (to be updated every semester by corresponding faculty member)

Name of teacher	Dima A. Sabbah, Ph.D.	Office Number	**227**
Phone number (extension)	31	Email	dima.sabbah@zuj.edu.jo
Office hours	Sun-Thurs (4-5 pm)		