Course Detailed Description – Procedures of the Course Plan Committee /Faculty of Pharmacy	**QF02/0408−2.1E**

Department	Pharmacy

Course Name	Drug Design	**Course No**.	201412
Prerequisite	201313, 201211, 201335	Credit Hours	
Number & date of course plan approval		Brief Description	See form QF02/0409

Course Objective	This course is designed to impart the knowledge in computational methods and drug design approaches. It will explore computational chemistry methods and their application in drug design. It is proposed to introduce the knowledge 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.
Intended Learning Outcomes	1. To emphasize on the general principles of drug design and drug action from an organic chemical perspective rather than from the perspective of specific classes. 2. To discuss new trends in drug discovery and development. 3. To be familiar in recent developments in key issues such as combinatorial chemistry, QSAR, recombinant technology, and molecular modeling. 4. To distinguish drug design approaches and their applications. To recognize computational methods categories and their applications.
Course Topics	1. Computational Chemistry 2. Conformational Analysis 3. Ligand-based drug design 4. Structure-based drug design 5. Combinatorial Chemistry 6. Quantitative Structure Activity Relationship

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Text Books	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. An Introduction of Medicinal Chemistry, 4th edition, Graham Patrick, Oxford Universtiy Press, 2008.
References	1- Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th edition, J. N. Delgado and W. A. Remers, Lippincott-Raven, 2011. 2- Burger's Medicinal Chemistry and Drug Discovery, 6th edition, M. E. Wolff, 2003. 3- The Organic Chemistry of Drug Synthesis, Vol. 1-6, D. Lednicer and L. A. Mitscher, John Wiley and Sons.
Grade Determination	1st Exam = 25% 2nd Exam = 25% Final Exam = 50%	Practical Course Grade Determination	Course Work = 50% (Reports, Term Papers, Quizes) Final Exam = 50%

Course Outline

Week	Hours	Subjects	Chapters in Textbook	Notes
1	1	**Molecular Modeling** - Computational Methods.	Textbook 1-3/	
2	1	**Molecular Modeling** - Potential energy. - Molecular mechanics	Textbook 1-3/	
3	1	**Molecular Modeling** - Quantum Mechanics - Conformational analysis	Textbook 1-3/	
4	1	**Molecular Modeling** - Molecular Dynamic Simulation (MD).	Textbook 1-3/	
5	1	**Molecular Modeling** - X-ray crystallography - Superposing	Textbook 1-3/	

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Week	Hours	Subjects	Chapters in Textbook	Notes
6	1	**Ligand-Based Drug Design** - Pharmacophore modeling	Textbook 1-3/	
7	1	**Structure-Based Drug Design** - Molecular Docking	Textbook 1-3/	
8	1	**Structure-Based Drug Design** - Molecular Docking Software	Textbook 1-3/	
9	1	**Combinatorial Chemistry** - General Aspects. - Parallel Synthesis. - Solid Phase Technique.	Textbook 1-3/	
10	1	**Combinatorial Chemistry** - Split synthesis: peptide libraries. - Anchors. - Protecting Groups.	Textbook 1-3/	
11	1	**Ligand-Based Drug Design** - Quantitative Structure-Activity Relationships (QSAR) - Methods to correlate physicochemical parameters with biological activity.	Textbook 1-3/	
12	1	**Ligand-Based Drug Design (QSAR)** - Equations and Graphs - Physicochemical Parameters - Hydrophobicity - Electronic Property - Steric Property	Textbook 1-3/	
Week	**Hours**	**Subjects**	**Chapters in Textbook**	**Notes**
13	1	**Ligand-Based Drug Design (QSAR)** - Hansch Analysis. - De Novo Method. - Enhancement Factor. - Topliss Schemes.	Textbook 1-3/	
14	1	**Ligand-Based Drug Design (QSAR)** - COMFA	Textbook 1-3/	
15	1	Practice on ChemDraw	Textbook 1-3/	

Approved by Dept. Chair		Date of Approval	

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Extra Information: (Updated every semester and filled by course instructor)

Course Instructor	Dima A. Sabbah, Ph.D.
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