



Course Detailed Description – Procedures of the Course Plan Committee /Faculty of Pharmacy	QF02/0408–1.0
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Department	Pharmacy
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Course Name	Drug Design	Course No.	201412
Prerequisite	Pharmaceutical organic chemistry-2 , Pharmacology-1-	Credit Hours	1
Number & date of course plan approval		Brief Description	See form QF02/0409

Intended Learning Outcomes	<ol style="list-style-type: none"> 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. Discussing new trends in drug discovery and development. Recent developments in key issues such as combinatorial chemistry, QSAR, recombinant technology and molecular modeling.
Course Topics	<ul style="list-style-type: none"> - Drug Discovery. - Lead Modifications. - Combinatorial Chemistry. - Quantitative Structure-Activity Relationships. - Correlation of Physicochemical Parameters with Biological Activity. - Computer-Based Methods of QSAR. - Ligand-based drug design. - Structure- based drug design. - Molecular Graphics-Based Drug Design. - Drug Discovery through Enzyme Inhibition.
Text Books	<ol style="list-style-type: none"> An introduction to Medicinal chemistry, 4th edition, Graham Patrick, Oxford University Press, 2008. The Organic Chemistry of Drug Design and Drug Action, 2nd edition, Richard B. Silverman, Elsevier, 2004. Foye's Principles of Medicinal Chemistry, 6th edition, Thomas L. Lemke and David A. Williams, Lippincott Williams & Wilkins, 2008.

References	<ol style="list-style-type: none"> 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	1 st Exam = 25% 2 nd Exam = 25% Final Exam = 50%			
Course Outline				
Week	Hours	Subjects	Chapters in Textbook	Notes
1 st	1	Molecular Modeling - Potential energy. - Molecular mechanics	17/1	
2 nd	1	Molecular Modeling - Potential energy. - Molecular mechanics	17/1	
3 rd	1	Molecular Modeling - Conformational analysis	17/1	
4 th	1	Molecular Modeling - X-ray crystallography	17/1	
5 th	1	Molecular Graphics-Based Drug Design - Docking. - Structure-based drug design.	17/1	
6 th	1	Molecular Graphics-Based Drug Design - Docking. - Structure-based drug design.	17/1	
7 th	1	Molecular Graphics-Based Drug Design - <i>de novo</i> design. -	17/1	
8 th	1	Quantitative Structure-Activity Relationships - Historical. - Steric effects: Taft equation. - Methods to correlate physicochemical parameters with biological activity.	18/1	
9 th	1	Quantitative Structure-Activity Relationships - Historical. - Steric effects: Taft equation. - Methods to correlate physicochemical parameters with biological activity.	18/1	



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10 th	1	Correlation of physicochemical parameters with biological activity <ul style="list-style-type: none"> - Hansch analysis. - De novo method. - Enhancement factor. - Topliss operational schemes. 	18/1	
11 th	1	Correlation of physicochemical parameters with biological activity <ul style="list-style-type: none"> - Hansch analysis. - De novo method. - Enhancement factor. - Topliss operational schemes. 	18/1	
12 th	1	Computer-Based Methods of QSAR: 3D-QSAR <ul style="list-style-type: none"> - CoMFA. 	18/1	
13 th	1	Combinatorial Chemistry <ul style="list-style-type: none"> - General aspects. - Split synthesis: peptide libraries. - Encoding combinatorial libraries. - Nonpeptide libraries. 	16/1	
14 th	1	Combinatorial Chemistry <ul style="list-style-type: none"> - General aspects. - Split synthesis: peptide libraries. - Encoding combinatorial libraries. - Nonpeptide libraries. 	16/1	
15 th	1	Practice on ChemDraw.	Practical	

Approved by Dept. Chair		Date of Approval	
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Extra Information: (Updated every semester and filled by course instructor)

Course Instructor	
Office No.	
Extension Email	
Office hours	