

Study program : Chemistry			
Type and level of studies: PhD studies of chemistry - BIOCHEMISTRY			
Course unit: Biochemistry of Physiologically Active Compounds			
Teacher in charge : Milan Mladenović, PhD, Associate Professor			
Language of instruction : English			
ECTS: 10			
Prerequisites: Entered PhD studies of chemistry - BIOCHEMISTRY			
Semester: Summer semester			
Course unit objective			
Student will be introduced with the term „Physiologically Active Compound”. Biochemical assays used in determination of activity of physiologically active compounds. Bioactive compound in physiological conditions and its activity. Introduction to the molecular modeling methods in biochemistry. Compound's interactions on protein and nucleic acids level. Bioactive conformation. Structure-activity relationships (SAR). Quantitative structure-activity relationships (QSAR). Three dimensional Quantitative structure-activity relationships (3-D QSAR). Pharmacophore. 3D Pharmacophore. Lead and hit compounds for design, future synthesis and evaluation.			
Learning outcomes of Course unit			
Recognition of chemical structures that bears biological activity. Chemical modification in order to enhance the activity (Bioisosters). Correlation of biological activity and physico-chemical parameters of compound (SAR, QSAR, 3-D QSAR). Molecular modeling of physiologically active compound on enzyme, receptor or DNA level. Rational Drug Design.			
Course unit contents			
<i>Theoretical classes.</i>			
The term pharmacophore. Structure-activity relationships (SAR). Quantitative Structure-activity relationships (QSAR). Inhibitor-enzyme interactions. Inhibitor-DNA interactions. Molecular modeling. Molecular docking. 3-D Pharmacophore. 3-D Quantitative Structure-activity relationships (3-D QSAR) CoMFA, CoMSIA, GRID methodology. Structure-based drug design. Ligand-based drug design. ADMETox and its predictions. Molecular dynamics.			
<i>Experimental classes</i>			
Competitive inhibition of enzyme reactions. QSAR model generations. RCSB Protein Data Bank survey for inhibitor-enzyme co-crystallized complexes (www.rcsb.org). Molecular docking using AutoDock, AutoDock Vina, DOCK6, PLANTS, and Paradocks. Molecular modeling with Schrödinger Suite. Ligand-based alignment using Baloon, Shaep, SurflexSim and Open3DAlign. SB and LB 3-D QSAR models using Sybyl Tripos. 3-D Pharmacophore using Discovery Studio. ADMETox features using Discovery Studio. Rational Drug Design.			
Literature			
1. G. Thomas, <i>Medicinal Chemistry</i> , John Wiley and Sons, Ltd. England, 2000.			
2. G. L. Patrick, <i>An Introduction to Medicinal Chemistry</i> , 4 th ed., Oxford University Press, England, 2009.			
3. Burger's <i>Medicinal Chemistry and Drug Discovery</i>			
4. Hugo Kubinyi, <i>3D QSAR in Drug Design: Volume 1: Theory Methods and Applications</i> , Springer Science & Business Media, 1993			
5. Hugo Kubinyi, <i>3D QSAR in Drug Design: Volume 2: Ligand-protein interactions and Molecular Similarity Theory Methods and Applications</i> , Springer Science & Business Media, 1995			
Number of active teaching hours			Other classes
Lectures: 5	Practice:	Other forms of classes: <i>mentoring system</i>	
Teaching methods			
Lectures, seminars, practical classes			
Examination methods (maximum 100 points)			
Exam prerequisites	No. of points:	Final exam	No. of points:
Student's activity during lectures	10	oral examination	
practical classes/tests	20	written examination	50
Seminars/homework	20	
Project			

Other			
Grading system			
Grade	No. of points	Description	
10	90-100	Excellent	
9	80-90	Exceptionally good	
8	70-80	Very good	
7	60-70	Good	
6	50-60	Passing	
5	<50	Failing	