

<b>Study Programme:</b> Master Academic Studies in Biochemistry			
<b>Course Unit Title:</b> Rational drug design			
<b>Course Unit Code:</b> IB-503			
<b>Name of Lecturer(s):</b> Professor Velimir Popsavin			
<b>Type and Level of Studies:</b> Master of Science Degree			
<b>Course Status (compulsory/elective):</b> elective			
<b>Semester (winter/summer):</b> winter			
<b>Language of instruction:</b> English			
<b>Mode of course unit delivery (face-to-face/distance learning):</b> Face-to-face			
<b>Number of ECTS Allocated:</b> 6			
<b>Prerequisites:</b> None			
<b>Course Aims:</b> Introduction to modern methods for the rational design of new biologically active molecules, potential drugs.			
<b>Learning Outcomes:</b> Upon successful completion of this course, the student is able to use the selected “Open Source” software for the rational drug design.			
<b>Syllabus:</b> <i>Theory</i> Chemical and biochemical databases of interest for the development of new drugs. Molecular recognition as the basis for rational drug design. Analysis of protein-ligand interactions. The process of drug design when the structure of the target protein is unknown and pharmacophore modelling. Examples of molecular mimicry of known drugs and biomolecules. Drug design when the structure of the target protein is known (structure-based design). Molecular docking and virtual screening. Rational design of HIV-1 protease inhibitors. <i>Practice</i> Identification and visualization of pharmacophore and ligand-receptor interactions in <i>Accelrys Discovery Studio Visualizer</i> and <i>Chimera</i> . Molecular docking using <i>AutoDock</i> and <i>AutoDock Vina</i> .			
<b>Required Reading:</b> 1. V. Popsavin: Rational drug design, internal script (ePMF), 2019. 2. D. C. Young: <i>Computational Drug Design</i> , John Wiley & Sons, Inc., Hoboken, 2009. 3. R. B. Silverman: <i>The Organic Chemistry of Drug Design and Drug Action</i> , 2 <sup>nd</sup> Ed., Elsevier, Amst., 2004. 4. <i>Software: Molecular Conceptor</i> , Ver. 2.15, Copyright 2001–1011, Synergix Ltd. www.drugdesign.com.			
<b>Weekly Contact Hours:</b> 75		<b>Lectures:</b> 30	
<b>Practical work:</b> 30+15			
<b>Teaching Methods:</b> Lectures, laboratory work, computer simulation, seminar(s)			
<b>Knowledge Assessment (maximum of 100 points):</b> 100			
<b>Pre-exam obligations</b>	points	<b>Final exam</b>	points
Active class participation	10	written exam	60

Practical work	20	oral exam	
Preliminary exam(s)		.....	
Seminar(s)	10		
The methods of knowledge assessment may differ; the table presents only some of the options: written exam, oral exam, project presentation, seminars, etc.			