Course code	MK202		
Course title	COMPUTATIONAL DESIGN OF BIOLOGICALLY ACTIVE MOLECULES		
General information			
Study programme	Graduate study „Drug research and development“, Graduate study „ Biotechnology in medicine“, Graduate study „Medical chemistry“	Academic year	
Lecturer	Doc. Dr. Sc. Željko Svedružić		
Status	**Required**	Elective	
ECTS system			**5**

Course objectives

The course aims to provide a thorough demonstration of the methods and computational packages used in the elucidation of structure and reactivity of biologically active molecules (potential drugs). In addition, the connection between experimental measurements and the results of molecular modelling calculations will be outlined, with special emphasis on enhancing the practical use of such computational methods in the students own research. The latter will be achieved by imparting a better understanding of the systems under investigation, with the goal of increasing the efficiency of connected experimental research.

Course description

The course will cover a variety of computational approaches applicable to the design of new biologically active molecules, with a focus on modeling the 3D structure of molecules and intermolecular interactions. This will include an overview of the computational methods and programs commonly used in the elucidation of structure and reactivity of potential drugs, including examples of empirical (molecular mechanics, molecular dynamics, MC, docking, and the discrete-point-space methodology) and quantum-mechanical (ab inito, HF, DFT and semi-empirical) techniques. In addition to clarifying the mathematical and physical principles underlying these methods, their application will be clearly demonstrated through carefully selected practical examples.

The connection with the laboratory will be highlighted through a comparison of selected experimental properties (X-ray and neutron diffraction, electron microscopy, and NMR, IR, and UV spectra) with those that can be obtained through modeling. In addition, attention will be given to the productive use of known results through the interaction with databases of, for example, macromolecular structures or the properties of small molecules.

Various examples will be drawn upon to demonstrate how the application of different statistical methods can establish, both qualitatively and quantitatively, the relationship between the structure and activity of molecular species. In particular, emphasis will be placed upon ways in which this information can be used, for example, to enhance the activity and/or diminish the toxicity of certain classes of compounds.

Learning outcomes

The students will become equipped with knowledge that will enable them to properly understand the results of molecular modelling investigations as well as to critically evaluate the modelling-related scientific literature. Becoming properly informed about the different modelling methods and their possibilities will assist the students in planning the appropriate application of such methods in the process of designing new biologically active molecules. Beyond this, the practical knowledge will consist of acquiring the ability to competently use at least one computational modelling software package, enabling the students to embark on preliminary modelling of the structures of small molecules alone. Importantly, successful candidates will also become comfortable in the use of molecular databases over the internet.