

Course code	MK103		
Course title	CHEMOMETRICS		
General information			
Study programme	Graduate study „Drug research and development“, Graduate study „Medical chemistry“	Academic year	
Lecturer	Doc. Dr. Sc. Katja Džepina		
Status	Required	Elective	
ECTS system			3
Course objectives			
To achieve competence in the statistical analysis of data, in the structural and electronic properties of molecules as well as their relationship with the physico-chemical properties and activities of molecules in the biological and environmental systems.			
Course description			
<p><i>General:</i> Structure, properties, activities and reactivity of molecules, Data-bases (search, quality of data, errors in data), Statistical modeling (classical numerical methods, multivariate analyses (PCA, PLS), Statistical design and tests, Model quality and chance correlations), Artificial intelligence methods. <i>Structural properties:</i> Molecular size and mobility parameters, Molecular volume and molecular surface (van der Waals model, solvent accessible surface, molecular surface and volume calculation), Electronic parameters and spectroscopic properties, Interactions of "small" molecules with large molecular systems. <i>Quantitative structure-property/activity relationships:</i> Molecular structure in gas-phase, solution and crystal, Thermodynamics and energy parameters of molecules in solutions, Free-Wilson model, Hansch model, Kamlet-Taft model, Theoretical analog of Kamlet-Taft model. <i>Application of quantitative modeling methods:</i> Quantitative estimation of molar properties (solubility and related properties, retention indexes), molecular reactivity/activity (radical reactions, inhibition of enzymatic activity), persistence and mobility of organic pollutants (soil sorption, abiotic degradation, biodegradation).</p>			
Learning outcomes			
To master the methods for statistical data analysis, the quantum-chemical methods in determining structural and electronic properties of molecules, the search of data-bases with molecular properties and activities, the developing of qualitative and quantitative structure-activity relationships models in drug design and environmental research.			
A3; A5; A8; B2; B5; C1; C3; C4			