

Study program: Integrated academic studies of Pharmacy			
Type and level of the study program: integrated academic studies			
Course title: QUANTUM CHEMISTRY (PhV-QUANT)			
Teacher: Mihalj M. Poša, Zita J. Farkaš-Agatić			
Course status: elective			
ECTS Credits: 3			
Condition: Organic chemistry I; Organic chemistry II			
Course aim Teach students about the theory of quantum chemistry that is used for calculating the density distribution of electrons in the molecule, and the parameters resulting from the distribution of electrons in order to be used as molecular descriptors			
Expected outcome of the course: Quantum nature of the distribution of electrons in multinuclear systems. Students will be able to independently using appropriate software to calculate molecular descriptors derived from the distribution of electrons.			
Course description <i>Theoretical education</i> 1. Wave function 2. Born Openchaimer approximation 3. Valence connection theory 4. Molecule orbit theory 5. Walsh diagram 6. Huckel method 7. Semi empirical methods 8. Ab inito methods 9. Application: Solvation Energy <i>Practical education: exercises, other forms of education, research related activities</i> Usage of proper software			
Literature <i>Compulsory</i> 1. Grant GH, Richards WG. Computational Chemistry, Oxford University Press, 1955 <i>Additional</i> /			
Number of active classes			Other:
Lectures: 30	Practice: 15	Other types of teaching: Research related activities:	
Teaching methods Lectures, practice			
Student activity assessment (maximally 100 points)			
Pre-exam activities	points	Final exam	points
Lectures		Written	
Practices		Oral	40
Colloquium		
Essay	60		