Study program: Integrated Academic Studies in Pharmacy	
Course title: Quantum Chemistry	
Teacher: Mihalj M. Poša, Zita J. Farkaš-Agatić, Kosta J. Popović	
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

Theoretical education

1. Wawe 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: Solvatation Energy

Practical education

Usage of proper software

Literature

Compulsory

1. Grant GH, Richards WG. Computational Chemistry, Oxford University Press, 1955

Number of active classes	**Theoretical classes:** 30	**Practical classes:** 15

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		