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

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: exercises, other forms of education, research related activities

Usage of proper software

Literature

Compulsory

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

Additional

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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		