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| **Study program:** Doctoral academic studies **-** Chemistry |
| **Course title:** Molecular Modeling in Organic Chemistry (H312C) |
| **Name of lecturer/lecturers:** Marija S. Genčić |
| **Type of course:** elective |
| **Number of ECTS allocated:** 10 |
| **Course objectives** Upgrading the acquired knowledge of PhD student in computer chemistry and the possibilities it provides for studying organic compounds and reactions. |
| **Course outcomes** Upon successful completion of this course, the student will be able to: - choose an appropriate theoretical model for solving a specific problem in organic chemistry,- perform geometry optimization and search the conformational space of the selected organic compounds and simulate its NMR, IR and UV/Vis spectra,- perform computer's prediction of selected properties of organic compounds, which will further enable them to predict differences in reactivity, i.e. activities within the appropriate set of compounds. |
| **SYLLABUS***Lectures*Computational chemistry: opportunities and limitations. Software. Application in the study of organic molecules. Different levels of theory. Choosing an appropriate theoretical model for study of organic molecules and reactions: molecular and quantum mechanics, Hartree-Fock method, basic sets, post Hartree-Fock methods and combined methods. Graphical models and feature maps of organic molecules: molecular orbitals, electron density, spin density and electrostatic potential. Modeling of vibrational frequencies and thermochemical properties organic molecules. Geometry optimization of organic molecules: equilibrium geometries. Conformational space of organic molecules. Transition states in organic reactions: retrieval and confirmation. Modeling of reaction energies. Simulation of NMR, IR and UV/Vis spectra of organic compounds using molecular modeling software. Molecular descriptors. QSAR (quantitative structure-activity relationship) analysis of organic compounds. |
| **References**1. S. Marković, Z. Marković, Molekulsko modeliranje, Centar za naučno-istraživački rad Srpske akademije nauka i umetnosti i Univerzitet u Kragujevcu, Kragujevac, 2012.2. F. Jensen, Introduction to computational chemistry (2nd Edition), John Wiley & Sons, Ltd., Chichester, England, 2007.3. N. L. Allinger, Molecular structure: Understanding steric and electronic effects from molecular mechanics, John Wiley & Sons, Ltd., Hoboken, New Jersey, 2010. |
| **Active teaching classes** | **Lectures:** 105 | **Laboratory work:** / |
| **Teaching mode:** lectures, seminar, consultations |
| **ASSESSMENT METHODS AND CRITERIA (Max 100 points)** |
| activity during the lecture - 10 points; seminar - 20 points; homework - 20 points; written exam - 50 points |