|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Study program:** Master studies Chemistry | | | | |
| **Course title:** Medicinal Chemistry (H225C) | | | | |
| **Name of lecturer/lecturers:** Marija S. Genčić | | | | |
| **Type of course:** elective | | | | |
| **Number of ECTS allocated:** 6 | | | | |
| **Course objectives**  Introducing students to the principles of medicinal chemistry and the synthesis of bioactive organic compounds. | | | | |
| **Course outcomes**  Upon successful completion of this course, the student is able to:  - propose synthesis methodology,  - achieve synthesis,  - and perform derivatization of previously designed organic compounds possessing pharmacophores. | | | | |
| **SYLLABUS**  *Lectures*  Biological and pharmacological activity. Activity testing. Biologically and pharmacologically active compounds. The term pharmacophore. Molecular design. Lead structure. Combinatorial chemistry. Creating a library of compounds. (Q)SAR analysis. Molecular descriptors. Topological indices. Molecular mechanics. Force fields. Geometry optimization. Conformational space. The importance of the availability of scientific information in the design and synthesis of new potentially biologically/pharmacologically active compounds - scientific search engines, journals and databases (SciFinder, NIST, Science Direct, Kobson, CCDC - Cambridge Crystallographic Data Centre, PDB - Worldwide Protein Data Bank, UniPro - Universal Protein Resource Knowledgebase). Strategies in the synthesis of biologically and pharmacologically active compounds. Chemo-, regio- and stereoselectivity (specificity). Total synthesis of selected biologically/pharmacologically active compounds: analysis and mechanisms of key steps in the synthesis and comparison of different approaches to the synthesis of a pharmacologically active compound/group of compounds. Analysis of the strategy applied in the synthesis of a selected library of compounds.  *Laboratory work*  Creation of a mini-library of potential biologically/pharmacologically active compounds: Molecular design. Retrosynthetic analysis. Synthesis planning. Literature search. Selection of reaction conditions. Synthesis of the selected compound from the created library. Purification and spectral characterization of the synthesized compound. Examination of interactions of synthesized compounds with selected enzymes and other biologically important macromolecules using standard spectrophotometric methods. (Q)SAR analysis of the created compound library. Optimizing the geometry/conformational space of selected compounds from the created library. | | | | |
| **References**  1. K. P. C. Volhard, N. E. Schore, Organska hemija, četvrto izdanje, Data status, Beograd, 2004.  2. M.B. Smith, J. March, Advanced Organic Chemistry: reactions, mechanisms, and structure (6th Edition), John Wiley and Sons Ltd., Hoboken, New Jersey, 2007.  3. Ž. Čeković, Organske sinteze: reakcije i metode, Zavod za udžbenike i nastavna sredstva, Beograd, 2006.  4. G. L. Patrick, An Introduction to Medicinal Chemistry (5th Edition), Oxford University Press, Oxford, United Kingdom, 2012.  5. D. Lednicer, L. A. Mitscher, 6 Volume Set, The Organic Chemistry of Drug Synthesis, Wiley-Interscience, New York, 1977.  6. A. W. Czarnik, S. H. DeWitt (Ed.), A practical guide to combinatorial chemistry, American Chemical Society, Washington, 1997.  7. A. Hinchliffe, Molecular modeling for beginners (2nd Edition), John Wiley and Sons Ltd., Chichester, England, 2008.  8. T. Pyzin, J. Leszczynski, M. Cronin (Ed.), Recent advances in QSAR studies: methods and applications. Springer, Dordrecht, Netherlands, 2010. | | | | |
| **Active teaching classes** | **Lectures 45** | | **Laboratory work 15** | |
| **Teaching mode:** lectures, interactive classes, laboratory exercises, seminars, consultations | | | | |
| **ASSESSMENT METHODS AND CRITERIA (Max 100 points)** | | | | |
| **Pre exam duties** | **Points** | **Final exam** | | **Points** |
| Activity during lectures | 5 | Written examination | | 40 |
| Practical teaching | 20 | Oral examination | |  |
| Teaching colloquia | 20 |  | |  |
| Seminar | 10 |  | |  |
| Homeworks | 5 |  | |  |