Table 5.2 Course description

<table>
<tr><td colspan="5">Study program: Chemistry, Master’s program, Module Cheminformatics and modelling</td></tr>
<tr><td colspan="5">Course title: Design of Bioactive Compounds</td></tr>
<tr><td colspan="5">Professor: Milan P. Mladenović</td></tr>
<tr><td colspan="5">Course type: Obligatory</td></tr>
<tr><td colspan="5">ECTS credits: 6</td></tr>
<tr><td colspan="5">Prerequisites: BSc degree in Chemistry or related sciences</td></tr>
<tr><td colspan="5">Course objectives
Introduction with the basic concepts of biomolecules activity as inhibitors and antagonists of biochemical reactions, related to their structure and pharmacology.</td></tr>
<tr><td colspan="5">Learning outcomes
Understanding of inhibitor-enzyme and antagonist-receptor interactions as a basis of inhibitors and antagonists consequent activity. Optimization of biomolecule’s structure, respecting the established interactions with the molecular target, by means of increasing the activity and alleviating the toxicity. The capability gained by student to plan the synthesis of novel bioactive compounds by means of rationality and efficacy.</td></tr>
<tr><td colspan="5">Course topics
Theoretical classes
The term and meaning of rational design of bioactive compounds. The criterions for selection of bioactive compounds. Classification of bioactive compounds according to the pharmacology, molecular targets and ATC system (anatomy, therapeutic and pharmacological features, chemical features). Computer-Aided Drug Design, CADD). Identification of molecular target: genetics, molecular biology, bioinformatics. Validation of molecular target: inhibitor-enzyme and antagonist-receptor interactions resolving by means of crystallography and NMR spectroscopy. Biological activity of molecules. Affinity, efficacy and potency of bioactive compounds. Essays for bioactivity determinations in in vitro and in vivo conditions. The in vitro-in vivo correlation. High Throughput Screening. The prediction biomolecules activity. Structure-Activity Relationships, SAR. Three-dimensional pharmacophore. Quantitative Structure-Activity Relationships, QSAR. Three-Dimensional Quantitative Structure-Activity Relationships, 3-D QSAR. Structure-Based Drug Design, SBDD. Ligand-Based Drug Design, LBDD. Hits and leads. Hit-to-lead optimisation. SOSA design of bioactive compounds. De novo design of bioactive compounds. SB и LB virtual screening.
Practical classes
Inhibitor-enzyme and antagonist-receptor complexes preparation by means of UCSF Chimera. Biomolecules preparation by means of MarvinSuite. Structure-Based alignment assessment and molecular docking by means of AutoDock, AutoDock Vina, DOCK, PLANTS, and ParaDocs. Ligand-Based alignment assessment and molecules structure comparison by means of Obconformer/Open3DALIGN and Balloon/ShaEP. 3-D QSAR studies by means of Py-CoMFA и Open3DQSAR. 3-D Pharmacophore generation by means of pharmACOphore.</td></tr>
<tr><td colspan="5">Recommended literature
1. Graham L. Patrick, An Introduction to Medicinal Chemistry, 4th ed., OxforD University Press, New York, USA, 2009.
2. Burger's Medicinal Chemistry and Drug Discovery by Donald Aberham, Volumes 1-6, A John Wiley and Sons, Inc., Publication, USA, 2003.
3. The Practice of MEDICINAL CHEMISTRY, edited by Camille Geogres Wermuth, Elsevier, Accademic Press, USA, 2003.</td></tr>
<tr><td colspan="4">Number of classes of active teaching</td><td>Other classes</td></tr>
<tr><td>Lectures:
2</td><td>Practicals:
2</td><td>Other forms of teaching:
Consultations</td><td colspan="2">Research work: 0</td></tr>
<tr><td colspan="5">Teaching methods
Problem-oriented teaching, practical training, seminar works, assignments.</td></tr>
<tr><td colspan="5">Knowledge assessment (maximum score 100)</td></tr>
<tr><td>Pre-exam obligations</td><td>points</td><td>Exam</td><td colspan="2">points</td></tr>
<tr><td>activity during the course</td><td>can influence the mark</td><td>written</td><td colspan="2">30</td></tr>
<tr><td>practical classes</td><td>10</td><td>oral</td><td colspan="2">20</td></tr>
<tr><td>colloquium(s)</td><td>20</td><td></td><td colspan="2"></td></tr>
<tr><td>Seminar(s)</td><td>20</td><td></td><td colspan="2"></td></tr>
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