Table 5.2 Course specification

Level: Bachelor

Course name: Medicinal Chemistry

Status: obligatory

ECTS: 8

Requirements: none

Course aim

Introduction to basic methods and biochemical principles relevant for the development, production and testing of biological activity of new pharmacologically active molecules - potential drugs.

Course outcome

Upon successful completion of this course, the student is able to: (1) define basic biochemical and chemical principles relevant to discovery of new drugs and to explain the importance of ligand-receptor interactions for drug action at the molecular level; (2) analyze structure-biological activity relationships and apply them to identify pharmacophores in known biologically active molecules; (3) explain the principles and importance of isosterism and bioisosterism for the design of analogues of known biologically active molecules; (4) understands and interprets the results of bioassays to determine antineoplastic activity in vitro.

Course content

Theory

Biochemical basis of drug action at molecular level. General principles for the development of new drugs. Brief overview of ligand-receptor interactions important for the pharmacological action of drugs at the molecular level. Biochemical principles for the development of new drugs. Stereochemistry and drug design. Solubility and drug design. Distribution and log P. Structural and biological activity (SAR) relationships: change in size and shape of molecules; alteration of existing ones and introduction of new substituents into the lead molecule (isosterism and bioisosterism). Quantitative structure-biological activity (QSAR) relationships. Biological tests for determination of antitumor activity. Application of stem cells in medicinal chemistry.

Practice: Practical classes, OFT, SRW

Laboratory exercises: multistep synthesis of pharmacologically active molecules and analogues; characterization of reaction intermediates and / or final products by spectroscopic methods. Introduction to experimental methods for determining the inhibition of neoplastic cell growth and for determining IC_{50} values. Computational exercises: identification and visualization of ligand-receptor interactions between selected drugs and biological macromolecules. Theoretical Calculations of Molecular Descriptors for QSAR Analysis.

Literature

G. L. Patrick: An Introduction to Medicinal Chemistry, 4th Edition, Oxford University Press, Oxford, 2009.
G. Thomas: Medicinal Chemistry – An Introduction, 2nd Edition, John Wiley & Sons, Ltd, Chichester, 2007.
T. Nogrady: Medicinal Chemistry: A Biochemical Approach, 2nd Edition, Oxford University Press, 1988.