Table 5.2 Course specification

Type and level of studies:Bachelor of Science Degree

Course name: Cheminformatics

Course status: elective

Number of ECTS credits: 6

Requirement: none

Course aim

Introduction to fundamental elements of cheminformatics as well as certain basic cheminformatic tools.

Course outcome

Upon successful completion of this course, students will be able to describe and apply fundamental cheminformatic methods and tools in solving diverse chemical problems.

Course content

Theory

Visualization and comparison of chemical structures (2D, 3D). Calculation of physico-chemical features of compounds. Structure descriptors. Databases. HTPS. Computer-aided drug design and spectral analysis. Molecular modelling. (Q)SAR. Computers and stereochemistry.

Practice: Practical classes, OFT, SRW

Introducing students to work with software for visualization of chemical structures as well as tools for their transformation from 2D to 3D. Discovering different formats of molecular data. Comparison of compounds based on their structure as well as physico-chemical features. Methods of data analysis and their application in computer-aided drug design, spectral analysis and molecular modelling. Prediction of potential drug reactivity based on their structure.

Literature

Popsavin, V.andSvirčev, M.*Cheminformatics*, internal script (ePMF)
Wegner, J. K.; Sterling, A.; Guha, R.; Bender, A.; Faulon, J.-L.; Hastings, J.; O'Boyle, N.; Overington, J.; Van Vlijmen, H.; Willighagen, E. *Commun. ACM***2012**, *55*, 65–75.
Chen, W. L. J. *Chem. Inf. Model.***2006**, *46*, 2230–2255.
Leach, A. R.; Gillet, V. J. *An Introduction to Chemoinformatics*; 2nd ed.; Springer, 2007.
Gasteiger, J.; Engel, T., Eds.; *Chemoinformatics: A Textbook*; 1st ed.; Wiley, 2003.
Bunin, B. A.; Siesel, B.; Morales, G.; Bajorath, J. *Chemoinformatics: Theory, Practice, & Products*; 1st ed.; Springer, 2007.

Number of classes of active teaching				Other classes
Lectures: 45	Practice: 30	OFT:	SRW:	

Teaching methods

Lectures, molecular modelling, seminar(s)

Assessment of knowledge (maximum of 100 points)

Pre-exam obligations	**Points**	Final exam	*points*
activity during lecture classes	10	written exam	60
practical teaching	20		
seminars	10		