

Table 5.2 Course description

Study program: Chemistry, Master's program			
Course title: Chemoinformatics			
Professor: Boris Furtula			
Course type: required			
ECTS credits: 5			
Prerequisites: BSc degree in Chemistry or related sciences			
Course objectives			
Chemoinformatics is new and dynamic area of chemistry that has been vigorously developed in recent years. The aim of this course is to introduce students with some of chemoinformatics' methods and tools applicable in various chemically related endeavors.			
Learning outcomes			
Students will be trained to use some of chemoinformatical methods in their own chemical projects.			
Course topics			
Chemistry and computers. Representation of 2D molecular structures. Chemical graph theory. Molecular generators. Molecular descriptors. Representation of 3D molecular structures. Chemical reactions in computers. From chemical data to chemical information. Classes of chemical data. Contemporary chemometrics' methods. Experimental design. Chemistry on the Internet. Structure and substructure searches. Applications of chemoinformatics. QSPR/QSAR.			
Recommended literature			
1. A. R. Leach, V. J. Gillet, <i>An Introduction to Chemoinformatics</i> , Springer, Dordrecht, 2007.			
2. J. Gasteiger (Ed.), <i>Handbook of Chemoinformatics – From Data to Knowledge</i> , Wiley, Weinheim, 2003.			
3. J. Bajorath (Ed.), <i>Chemoinformatics – Concepts, Methods, and Tools for Drug Discovery</i> , Humana Press, Totowa, 2004.			
4. R. Todeschini, V. Consonni, <i>Molecular Descriptors for Chemoinformatics</i> , Wiley, Weinheim, 2009.			
5. I. Gutman, <i>Uvod u hemijsku teoriju grafova</i> , PMF Kragujevac, Kragujevac, 2003.			
6. P. Gemperline (Ed.), <i>Practical Guide to Chemometrics</i> , Taylor & Francis, Boca Raton, 2006.			
Number of classes of active teaching			Other classes
Lectures: 2	Practicals: 2	Other forms of teaching: Consultations	
Teaching methods			
Problem-oriented teaching, practical training, seminar works, assignments.			
Knowledge assessment (maximum score 100)			
Pre-exam obligations	points	Exam	points
activity during the course	can influence the mark	written	30
practical classes	10	oral	30
colloquium(s)			
Seminar(s)	30		