

<b>Course title:</b> Chemoinformatics			
<b>Professor:</b> Boris Furtula			
<b>Course type:</b> optional			
<b>ESPB credits:</b> 10			
<b>Prerequisites:</b> Basic knowledge of mathematics and organic chemistry. Knowing of elements of computer science is not mandatory but it is preferable.			
<b>About course:</b> Chemoinformatics is an area of chemistry that has vigorous growth in recent few decades. The aim of this course is to introduce students with some elementary chemoinformatics' methods and tools that can be applied for solving diverse chemical problems.			
<b>Goal of the course:</b> The ultimate goal is the training of students to use chemoinformatics tools in their own projects.			
<b>Syllabus:</b> 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.			
<b>Recommended literature:</b>			
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.			
<b>Activity</b>	<b>Lectures:</b> 5 per week		
<b>Type of lecturing:</b> Classical lecturing, students' essays.			
<b>Examination (total number of points 100)</b>			
<b>Pre-exam activities</b>	<b>Points</b>	<b>Final exam</b>	<b>Points</b>
Activity in class	10	Written examination	30
Student essays	40	Oral examination	20