



УНИВЕРЗИТЕТ У БАЊОЈ ЛУЦИ  
UNIVERSITY OF BANJA LUKA  
ПРИРОДНО-МАТЕМАТИЧКИ ФАКУЛТЕТ  
FACULTY OF NATURAL SCIENCES AND MATHEMATICS



CHEMISTRY DEPARTMENT

Ph.D. STUDIES

Course name	Selected Chapters of Chemical Informatics			
Course code	Course status	Semester	Hours of instruction	ECTS
HEM23OPI	elective	I, II, III, IV	5+0	10
Teacher(s)	Prof. Dragan Matić, PhD, Milana Grbić, PhD			

Prerequisite course(s)	Entry requirements
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**Course goals**  
The goal of the course is for students to master the methods for presenting, manipulating, analyzing, and synthesizing chemical information necessary for the student's scientific research work.

**Learning outcomes**  
The student:  
Understands the principles of different representations of molecules. Distinguishes and uses different formats to represent information about chemical structures. Selects the most suitable formats for the representation of chemical reactions for the application of various computer tools. Uses various computer tools to process chemical information. It uses programming techniques to manipulate chemical data. Manipulates databases that store information about chemical structures and their relationships. Uses artificial intelligence techniques to extract useful information from chemical data.

**Course content**  
\*Principles of molecular representation: Chemical and mathematical notation, Specific types of chemical structures, Spatial representation of chemical structures.  
\*Computer processing of information on chemical structures: Standard formats of information on chemical structures, Chemical structures as input/output data, Processing of 3D structural information.  
\*Computer processing of information about chemical reactions: Types of reactions, Equations of reactions, Learning from information about chemical reactions, Databases about chemical reactions, Classification of chemical reactions.  
\*Data: Data Types, Data Storage and Data Management.  
\*Databases and data sources in chemistry: Basic systems of chemical databases, Databases of compounds, Reaction databases.  
\*Search for chemical structures: Search for complete structures, Search for parts of structures, Search for similar structures, Search for 3D structures, Search for protein and amino acid sequences.

**Teaching methods**  
Consultative teaching

**Books and other learning materials**  
1. Engel, Thomas, and Johann Gasteiger, eds. Chemoinformatics: basic concepts and methods. John Wiley & Sons, 2018.  
2. Varnek, Alexandre, ed. Tutorials in chemoinformatics. John Wiley & Sons, 2017.

**Course activities and grading method**  
Research work, final exam

Research work	40	Final exam	60
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**Additional course notes**

Name of the teacher who prepared this form	Dragan Matić, Milana Grbić
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