

Level: Bachelor				
Course title: Application of computers in chemistry (IH-101)				
Status: Elective				
ECTS: 5				
Requirements: none				
Learning objectives The aim of the course is to train students for independent computer use when writing term papers in chemistry, drawing graphics or chemical structures and processing experimental data.				
Learning outcomes After finishing the course, student will be able to: • write term papers using modern computer programs for processing of the text, files, formulas and equations • successfully process obtained experimental data by regression analysis • graphically present the structure and conformations of different molecules				
Syllabus Applications MS Word for Windows for text processing, Math Type and text processing with a special chemical symbols and chemical equations. Training students to write term papers. MS Excel: a spreadsheet, using functions, solving problems using tables. Draw different types of graphics and features that are commonly used in chemistry. Program Origin and processing of the experimental data. Calculations and fitting of experimental data. Regression analysis. Programs for plotting molecular and structural formula, ChemSketch, ChemDraw. Inserting drawn graphics including images and graphics to text. Displaying three-dimensional structure of molecules and 3-D graphics. Optimization of the structure and geometry of molecules. Conformational analysis of small molecules. Databases in chemistry. The practical part of the course is an integral part of the course and includes practical use of computers for writing and processing of the text, graphics and pictures in chemistry.				
Weekly teaching load				Other:
Lectures: 2	Exercises: 2	Other forms of teaching: /	Student research: /	