

Table 5.2 Course description

Study program: Chemistry, Master's program, Module Cheminformatics and modelling			
Course title: Linux in Chemistry			
Professor: Milan P. Mladenović			
Course type: Electoral			
ECTS credits: 5			
Prerequisites: BSc degree in Chemistry or related sciences			
Course objectives Introduction with the Linux (Unix) operative system as a multifunctional platform with the wide application in science. Application of Linux in chemistry and usage of Linux-based molecular modelling programs.			
Learning outcomes The skills gained by student to use Linux environment for performing experimental protocols in chemistry.			
Course topics <i>Theoretical classes</i> Work with terminal and Bash (<i>i.e.</i> the Bourne Again Shell) command line as an interface for managing the Linux operating system. The structure of Linux syntax. The chemical molecule as a textual file. Work with text editors (vim, nano, emacs, ect.) by means of chemical compounds structures consideration and manipulation. Chemical format structures: PDB, MOL2, SDF, SMILE and other formats. Basic Linux commands for text editing and manipulation (<i>i.e.</i> the improvement of molecule's structure): cat, grep, sed, sort, head, tail ect. Molecule's file format conversion by means of OpenBabel toolkit. The adjustment of chemical structure according to the reaction conditions by means of OpenBabel toolkit. Molecule's structural features by means of OpenBabel toolkit: conformational analysis, calculation of conformers' energies, definition of local and global minima. Force field file format as a basis for calculation of physic-chemical parameters on personal computer. Molecular graphic softwares by means of command line application: UCSF Chimera и VMD. Work with a large number of compounds. Basic and intermediate Bash scripting and molecular modelling automatization. The structure of Bash scripts. The concept of lists and variables and its application. Logical loops for, if, elif, while, until and their application. Bash functions and their application. Generation of user's own commands and configuration files. Debugging of Bash scripts by means of shellcheck tool. <i>Practical classes</i> The application of theoretical knowledge on various chemical problems.			
Recommended literature 1. William E. Shotts, Linux from command line. A complete Introduction. ebook, ISBN-10/ASIN: 1593273894 ISBN-13: 978-1593273897 2. Ellen Siever, Stephen Figgins, Robert Love, Arnold Robbins, LINUX in a nutshell, 6 th ed., O'RELLY Media, USA, 2009. 3. Chris F. A. Johnson, Pro Bash Programming. Scripting the GNU/Linux Shell, Apress, Springer-Verlag New York, Inc., USA, 2009. 4. Learning the bash shell, 3 rd ed. O'RELLY Media, USA, 2009.			
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	20
colloquium(s)	20		
Seminar(s)	20		