

Table 5.2 Course description

Study program: Chemistry, Master's program			
Course title: Python for chemists			
Professor: Boris Furtula			
Course type: required			
ECTS credits: 5			
Prerequisites: BSc degree in Chemistry or related sciences			
<p>Course objectives</p> <p>Computers are nowadays inevitable in any serious research endeavors. Boosting and automation of hard and non-creative jobs represents the main power of computers in daily scientific routines. A need for developing a software for some specific job in chemical investigations is not quite rare. Therefore, a knowledge of at least one programming language is desirable. The main objective of this course is to introduce students with some elements of Python programming applied on examples taken from real-life chemistry problems.</p>			
<p>Learning outcomes</p> <p>It is expected that after this course, students will be able to participate in developing small and medium Python programming projects, which will automatize some laboring chemistry routines.</p>			
<p>Course topics</p> <p>Why Python; installation and setup of Python; first Python program; conversation with Python shell; variables and types of variables; name convention of variables and keywords; Python phrases; Operators; Python comments; if-statements; exceptions; loops; functions; io-operations; data in Python; tuples; lists; dictionaries; visualizations of data; chemically interesting modules in Python.</p>			
<p>Recommended literature</p> <ol style="list-style-type: none"> 1. C. Severance, <i>Python for Informatics</i>, www.dr-chuck.com. 2. Z. A. Shaw, <i>Learn Python the Hard Way</i>, https://learnpythonthehardway.org/. 3. J. M. Stewart, <i>Python for Scientists</i>, Univ. Cambridge, Cambridge, 2014 			
Number of classes of active teaching			Other classes
Lectures: 2	Practicals: 2	Other forms of teaching: Consultations	
<p>Teaching methods</p> <p>Problem-oriented teaching, practical training, seminar works, assignments.</p>			
Knowledge assessment (maximum score 100)			
Pre-exam obligations	points	Exam	points
activity during the course	can influence the mark	written	30
practical classes	30	oral	20
colloquium(s)			
Seminar(s)	20		