

Course title in English	Script programming languages
Course title in Polish	Języki skryptowe
Course code	
Type of course	Lecture
Level of course	PhD
Year of study	1-4
Semester/trimester	2/4/6/8
Number of hours/credits allocated	30/2
Name of lecturer	Cezary Czaplewski
Objective of the course (expected learning outcomes and competences to be acquired)	<u><i>Knowledge:</i></u> Recognition and characterization of shells used on unix systems (bash, tcsh), scripting tools for text processing (sed, awk), Tcl and Python languages, as well as Tcl/Tk and Python/Tkinter based graphic libraries. Knowledge of the usefulness of known data processing tools and their application in scientific calculations. <u><i>Skills:</i></u> Solving simple programming problems using scripts. Application of selected script languages in independent implementation of own projects. <u><i>Social competence:</i></u> Group work, the ability to participate in constructive discussions.
Prerequisites	Completed the course of Information technology
Course contents	Script programming languages are widely used in scientific calculations, data presentation and data processing. The aim of the course is to develop the skills necessary to solve simple programming problems using script languages. The course includes the following subjects:

	1. Use of shells on unix systems (bash, tcsh) for writing scripts. 2. Processing of text files in the sed stream editor. 3. Introduction to the awk programming language. 4. Introduction to scripts in Tcl language. 5. Python - an object oriented scripting language. 6. Tk graphic library, simple GUI design using Tcl/Tk and Python/Tkinter.
Recommended reading	1. A. Robbins, N.H.F. Beebe, Programowanie skryptów powłoki. Helion, 2005 2. A. Robbins, Sed i awk. Helion, 2002 3. D. Chrobak, Tcl-Tk. Programowanie, Helion, 2003 4. M. Lutz, Python. Wprowadzenie, Helion, 2009
Teaching methods	Lecture with multimedia presentation
Assessment methods	Solving programming assignments during the semester, final exam.
Language of instruction	Polish
Course title in English	Structural problems of biologically active compounds
Course title in Polish	Strukturalne zagadki związków biologicznie czynnych
Course code	
Type of course	Lecture
Level of course	PhD
Year of study	1-4
Semester/trimester	2/4/6/8
Number of hours/credits allocated	15/1
Name of lecturer	dr hab. Artur Sikorski, Professor UG
Objective of the course (expected learning outcomes and competences to be acquired)	<u>Knowledge:</u> Student: has basic knowledge in the field of X-ray methods and the possibilities of their use in order to identify biologically active compounds; knows the general idea of X-ray diffraction measurements; knows how to determine the crystal structure of biologically active compounds; knows how to interpret the powder spectrum; knows how to interpret experimental data obtained as a result of X-ray

	methods; knows the advantages and disadvantages of X-ray methods used to identify biologically active compounds; knows the basic bases of crystal structures for small and large molecules of biologically active compounds, knows how to use them and what structural data can be obtained from them. <u>Skills:</u> Student: • organizes workshop. • solves scientific problems, critically refers to the results obtained, • proposes alternative methods of solving scientific problems, • analyzes the results obtained based on their knowledge, • draws conclusions based on experimental data, • verifies the results based on literature data <u>Social competence:</u> Student: • strives to acquire knowledge, • works independently, and in a team performing different roles in it, • shows creativity during the presentation of results, • engages in solving scientific problems, • cares for the acquisition of knowledge by others, • discusses scientific problems (theses)
Prerequisites	completed courses in "General chemistry" and "Physical chemistry"
Course contents	Is the structure of biologically active compounds in the 21st century a problem for a chemist? The role of X-ray methods in modern chemistry. The idea of X-ray measurements. Apparatus used for X-ray diffraction experiments (single crystals and powders). Solving and refinement of the crystal

	structure and interpretation of structural data for small- and large molecules of biologically active compounds. Preparation and interpretation of spectra of powdered biologically active compounds. Determination of the absolute configuration of biologically active compounds. Basic crystallization techniques. Correlation between structure and biological activity of biologically active compounds. Inter- and intramolecular interactions in crystals. Crystallographic structural databases and bases of powder diffraction data - the possibilities of their use during the interpretation of experimental data obtained as a result of X-ray measurements carried out for biologically active compounds. Application of X-ray diffraction methods in various fields of industry and science.
Recommended reading	A. Literature required to pass the course 1. Bojarski Z., Gigla M., Stróż K., Surowiec M., Krystalografia, PWN, 2008. 2. Trzaska Durski Z., Trzaska Durska H., Podstawy krystalografii strukturalnej i rentgenografii, Oficyna Wydawnicza. Politechniki Warszawskiej, 2003. 3. Atkins P. Chemia fizyczna, PWN, 2016. B. Extracurricular readings 1. Penkala, T., Zarys Krystalografii, PWN, 1983. 2. Luger, P., Rentgenografia strukturalna monokryształów, PWN, 1989. 3. Wells, A. F., Strukturalna chemia nieorganiczna, WNT, 1993. 4. Scientific articles
Teaching methods	Lecture (multimedia presentation)
Assessment methods	A. Final evaluation, in accordance with the UG study regulations exam for a grade B. Assessment methods written exam - test containing open and closed questions

	C. The basic criteria for evaluation or exam requirements • a test exam consisting of 20-25 open and closed questions, covering issues mentioned in the lecture's program content; • final grade according to the scale of grades given in the Study Regulations • additional written exam for students who did not obtain the required 51% in the first term
Language of instruction	Polish