Zał. nr 5 do ZW 78/2023

Attachment no. 4. to the Program of Studies

FACULTY of CHEMISTRY

SUBJECT CARD

Name of subject in Polish *Informatyka dla inżynierów*
Name of subject in English *Informatics for engineers*
Main field of study (if applicable): …….
Specialization (if applicable): ……..
Profile: academic / ~~practical~~*
Level and form of studies: ~~1st~~/ 2nd level, ~~uniform magister studies~~*, full-time / ~~part-time~~*
Kind of subject: obligatory / ~~optional / university-wide~~*
Subject code W03W03-SM2018L
Group of courses ~~YES~~ / NO*

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)			30		
Number of hours of total student workload (CNPS)			50		
Form of crediting (Examination / crediting with grade)			crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points			2		
including number of ECTS points for practical classes (P)			2		
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)			1,4		

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of general chemistry, linear algebra, mathematical analysis;
2. Basic knowledge of computer science;
3. Specialized English.

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SUBJECT OBJECTIVES

C1 Introducing main chemical, biological and bibliographic databases.
C2 Teaching about basic formats used in chemical and bioinformatic databases.
C3 Introducing software used for drawing and visualization of chemical structures and macromolecules.
C4 Teaching students the basics of the scripting language.
C5 Teaching students the skills allowing the automation of computational tasks.

SUBJECT EDUCATIONAL EFFECTS

relating to skills:
PEU_U01 – ability to search chemical and bibliographic databases and biological sequences databases;
PEU_U02 – ability to use chemical structures visualization tools;
PEU_U03 – ability to select appropriate methods and tools for the studied problem;
PEU_U04 – ability to develop an algorithm;

PEU_U05 – ability to use a scripting language to automate computational tasks and solve simple numerical problems.

PROGRAMME CONTENT

Laboratory		Number of hours
Lab 1	**Introductory classes**: the program of laboratory classes, organization and rules of the computer lab, grading rules. Introduction of basic tools and software used during the course.	2h
Lab 2 & Lab 3	**Scientific databases**: introduction to the selected chemical, scientific and bibliographic databases (e.g. Reaxys, ChemSpider, CSD, PDB, Scopus, WoS, NCBI), data organization and presentation, search options. The importance of obtaining scientific information from reputable and verified sources will be discussed.	4h
Lab 4	**Data formats and visualization of molecule structures:** introduction to data formats used in chemical and structural databases and the formats used for biological sequences. Practical exercises on searching for information in chemical databases. Practical examples of the use of visualization software and tools used for building of molecular structures.	2h
Lab 5	Individual Project I	2h
Lab 6	**Introduction to Python**. Introduction of numerical data types and arithmetic operators. The first scripts - working with numerical data and using arithmetic operators. Introduction of interactive Python.	2h
Lab 7	**Basic data types**. Overview of basic data types: numbers and strings. Writing scripts that use data provided by the user. Practical examples of using Help.	2h
Lab 8	**Conditional statement**. Overview of the principles of creating conditional statements and creating a group of statements. Practical examples e.g. calculating factorials, printing a multiplication table.	2h
Lab 9	**Advanced data types** - lists, tuples, dictionaries. Creating lists, tuples and dictionaries as well as introduction of their operators and methods. Writing scripts using these data types. Programming test I.	2h
Lab 10	**While loop**. Overview of the principles of creating loops controlled by a logical condition together with practical examples.	2h
Lab 11	**Modules**. The rules of importing modules and their use in practice (math and random module). Practical exercises with a while loop.	2h
Lab 12	**For loop**. Overview of the principles of creating a counter controlled loop. Programming test II.	2h
Lab 13	**Counter controlled loop**. Practical examples of scripts using counter-controlled loops, exercises with complex instructions and loop control statements.	2h
Lab 14	**Text Files**. Overview of processing of text files. Exercises using biological sequences.	2h
Lab 15	Programming test III. Repetition of tests I and II. Discussion of Individual Project.	2h
	Total hours	30h

TEACHING TOOLS USED

N1. Lecture/presentation
N2. Scripts writing
N3. Practical usage of databases
N4. Practical usage of software
N5. Solving the exercises

N6. Preparation of reports

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming during semester), P – concluding (at semester end)	Learning outcomes code	Way of evaluating learning outcomes achievement
F1	PEU_U01-PEU_U03	Report from the Individual Project I
F2	PEU_U03-PEU_U05	Programming test I
F3	PEU_U03-PEU_U05	Programming test II
F4	PEU_U03-PEU_U05	Programming test III
P = (F1 + F2 + F3 + F4)/4		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] Python 3 documentation: https://docs.python.org/3/
[2] Python Crash Course, 3rd Ed.: A Hands-On, Project-Based Introduction to Programming, Matthes E., No Starch Press, 2023
[3] Python Programming: An Introduction to Computer Science, Zelle J. Ingram short title, 2016

SECONDARY LITERATURE:

[1] Python Programming for Beginners, Robbins P., 2023

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

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