FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in Polish: Informatyka chemiczna
Name of subject in English: Chemical informatics
Main field of study (if applicable): Chemistry and Industrial Analytics*
Specialization (if applicable):
Profile: academic
Level and form of studies: 1st level*, 2nd level – supplementary semester, full-time
Kind of subject: obligatory
Subject code: INC014001, INC024009
Group of courses: NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)			30		
Number of hours of total student workload (CNPS)			60		
Form of crediting			Crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points			2		
including number of ECTS points for practical (P) classes			2		
including number of ECTS points for direct teacher-student contact (BK) classes			1		

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

SUBJECT LEARNING OUTCOMES

C1 Introducing the Linux operating system
C2 Introducing main chemical and biological databases.
C3 Teaching about the formats used in chemical and sequence databases.
C4 Introducing software used for drawing and visualization of chemical structures.
C5 Teaching students the basics of the scripting language.
C6 Teaching students the skills allowing the automation of computational tasks.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:
PEK_W01 - knowledge of the basic chemical and biological databases,
PEK_W02 - knowledge of the formats used in chemical databases and databases of biological sequences,
PEK_W03 - knowledge of the software used for chemistry and its applications,
PEK_W04 - knowledge of the principles of algorithms design and main rules and expressions in the script language,
relating to skills:
PEK_U01 - ability to use the Linux operating system,

PEK_U02 - ability to search chemical databases and biological sequence databases,
PEK_U03 – ability to select appropriate methods and tools for the studied problem,
PEK_U04 - ability to use chemical structures visualization tools,
PEK_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. Introduction of basic tools and software used during the course. Introduction to the Linux operating system.	2h
Lab 2	**Chemical databases**: introduction to the main chemical and scientific databases (e.g. CSD, PDB, Reaxys, Scopus, NCBI), data organization and presentation.	2h
Lab 3	**Data formats in chemical databases**. Introduction the data formats used in chemical and structural databases and the formats used for biological sequences. Practical exercises on searching for information in chemical databases.	2h
Lab 4	**Visualization of chemical structures**. Introduction of the chemical structures visualization software and tools used for building of molecular structures, e.g. Molden.	2h
Lab 5	Individual Project I	2h
Lab 6	**Introduction to Python**. Introduction of numbers data types and arithmetic operators. The first scripts - working with numerical data and using arithmetic operators (e.g. energy units conversion). Introduction of interactive Python.	2h
Lab 7	**Basic data types**. Overview of basic data types: numbers and strings. Writing scripts that process 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 a loop controlled by a logical condition together with practical examples.	2h
Lab 11	**Modules**. The rules of modules import 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 programs using counter-controlled loops and complex examples requiring compound instructions.	2h
Lab 14	**Text Files**. Overview of text files processing. 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
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 number	Way of evaluating learning outcomes achievement
F1 (Laboratory)	PEK_W01- PEK_W03, PEK_U01-PEK_U04	Report from the Individual Project I
F2 (Laboratory)	PEK_W03- PEK_W04, PEK_U01, PEK_U03,PEK_U05	Programming test I
F3 (Laboratory)	PEK_W03- PEK_W04, PEK_U01, PEK_U03, PEK_U05	Programming test II
F4 (Laboratory)	PEK_W03- PEK_W04, PEK_U01- PEK_U03, PEK_U05	Programming test III

C (Laboratory) **=F1+F2+F3+F4**

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] *Python Crash Course,* Matthes E. No Starch Press, 2015

SECONDARY LITERATURE:

[1] http://docs.python.org
[2] *Think Python: How to Think Like a Computer Scientist, 2nd edition*, A. B. Downey, O'Reilly, 2015
[3] *Beginning the Linux Command Line,* S. Vugt. Springer, 2009
[4] *A Primer on Scientific Programming with Python,* H. P. Langtangen, Springer, 2011

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

Renata Grzywa, PhD, renata.grzywa@pwr.edu.pl