FACULTY of Chemistry
Wrocław University of Technology

SUBJECT CARD

Name in Polish **Programowanie zaawansowane i metody numeryczne**

Name in English **Advanced Programming and Numerical Methods**

Main field of study (if applicable): biotechnology
Specialization (if applicable): bioinformatics
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code INC024003
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		

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of linear algebra
2. Basic knowledge of mathematical analysis (conforming to the standard of the course „Analiza matematyczna 1")
3. Knowledge of Python scripting language (Applied Informatics course)

SUBJECT OBJECTIVES	
C1	Advanced techniques of programming, including optimization of the code.
C2	Introduction to numerical methods used in science and engineering.

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

The student -

PEK_W01 – knows basic numerical methods used in science and engineering.

Relating to skills:

The student -

PEK_U01 – is able to solve advanced numerical problems using scripting language.

PEK_U02 – is able to write failproof, efficient and fast programs.

Form of classes - laboratory		Number of hours
Lab 1	Introductory class.	2
Lab 2	Simple simulation script using Python.	2
Lab 3	Floating point representation; using Taylor's expansion.	2
Lab 4	Numerical differentiation and integration.	2
Lab 5	Random number generators.	2
Lab 6	Finding roots; polynomials.	2
Lab 7	Solving sets of linear equations.	2
Lab 8	Linear regression and interpolation.	2
Lab 9	Linear algebra.	2
Lab 10	Discussion of the first assignement.	2
Lab 11	Optimization techniques.	2
Lab 12	Numerical stability and condition number.	2
Lab 13	Solving differential equations.	2
Lab 14	Code optimization and efficient programming.	2
Lab 15	Discussion of the individual assignements.	2
	Total hours	**30**

TEACHING TOOLS USED	
N1	sample program discussion
N2	writing a program
N3	using existing software
N4	individual assignement

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1 (laboratory)	PEK_U01	Assignement 1
F2 (laboratory)	PEK_W01, PEK_U02	Assignement 2
C (laboratory) = 3,0 if (F1 + F2) = 11-12 points. 3,5 if (F1 + F2) = 13-14 points. 4,0 if (F1 + F2) = 15-16 points. 4,5 if (F1 + F2) = 17-18 points.		

	5,0 if (F1 + F2) = 19-20 points. 5,5 if (F1 + F2) = 19-20 points and F1, F2 were solved using techniques significantly exceeding the course program.

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] H. P. Langtangen. A Primer on Scientific Programming with Python (Springer, 2011) ISBN: 978-3-642-18365-2 http://link.springer.com/book/10.1007/978-3-642-18366-9/page/1

[2] T. Pang, Metody obliczeniowe w fizyce (PWN 2001), ISBN: 83-01-13511-5

SECONDARY LITERATURE:

[1] A. B. Downey. Python for Software Design: How to Think Like a Computer Scientist (Cambridge University Press, 2009), 1st edn. ISBN: 978-0521725965. http://www.greenteapress.com/thinkpython/index.html

[2] M. Pilgrim. Dive Into Python (Apress, 2004), 1st edn. ISBN: 978-1590593561. http://www.diveintopython.net

[3] K. D. Lee. Python Programming Fundamentals (Springer, 2011) ISBN: 978-1-84996-536-1 http://link.springer.com/book/10.1007/978-1-84996-537-8/page/1

[4] J. F. Epperson, An Introduction to Numerical Methods and Analysis (Wiley 2002) ISBN: 0-471-31647-4

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT
Advanced Programming and Numerical Methods
AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY
Biotechnology

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
PEK_W01	S2Abt5_U12	C2	La1-La13	N1-N4
PEK_U01	S2Abt5_U12	C2	La1-La13	N1-N4
PEK_U02	S2Abt5_U12	C1	La14-La15	N1-N4

** - enter symbols for main-field-of-study/specialization educational effects
*** - from table above

FACULTY of Chemistry
Wrocław University of Technology

SUBJECT CARD

Name in Polish **Informatyka stosowana**
Name in English **Applied informatics**
Main field of study (if applicable): biotechnology
Specialization (if applicable): bioinformatics
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code INC024006
Group of courses NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)			60		
Number of hours of total student workload (CNPS)			120		
Form of crediting			crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points			4		
including number of ECTS points for practical (P) classes			4		
including number of ECTS points for direct teacher-student contact (BK) classes			2		

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge od linear algebra
2. Basic knowledge of mathematical analysis (conforming to the standard of the course „Analiza matematyczna 1")

SUBJECT OBJECTIVES	
C1	User-level skills in the Linux operating system.
C2	Practical knowledge of the Python scripting language and ability to automate various tasks typical to bioinformatics using computer.
C3	Techniques of automated and routine production of graphs and data visualisation.
C4	Basic understanding and working knowledge of SQL (based on MySQL).

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

The student -

PEK_W01 – has general knowledge of structural and object-oriented programming; understands terms such as variable, type, function, operator, class, instance andinheritance. Knows how to use conditional statement, loops; knows how to read and write text files.

PEK_W02 – has basic knowledge of SQL language.

Relating to skills:

The student -

PEK_U01 – is able to use the Linux operating system.

PEK_U02 – is able to utilize a scripting language to automate his work and is able to write script for processing large amounts of data in a routine manner.

PEK_U03 – knows how to represent data using graphs and how to automate this process.

PEK_U04 – is able to build SQL queries in order to create and manage databases.

Form of classes - laboratory		Number of hours
Lab 1	Introductory class; command line and programs in Linux.	4
Lab 2	Simple Python scripts: reading and printing text, numerical data conversion. Interactive Python.	4
Lab 3	Using conditional statement: finding roots of a squaring function.	4
Lab 4	Working with condition-controlled loops.	4
Lab 5	Using count-controlled loops to compute factorial and sum of series. Printing multiplication table.	4
Lab 6	Writing scripts to process text files.	4
Lab 7	Using regular expressions.	4
Lab 8	Launching external programs from Python scripts.	4
Lab 9	Evaluation of the first assignement.	4
Lab 10	Introduction to numpy module.	4
Lab 11	Creating graphs in Python using supplied data.	4
Lab 12	Applications of the scipy module.	4
Lab 13	Basics of SQL language.	4
Lab 14	Using SQL in Python scripts.	4
Lab 15	Test correction and discussion of the individual assignements.	4
	Total hours	**60**

TEACHING TOOLS USED	
N1	sample program discussion
N2	writing a program
N3	using existing software
N4	individual assignement

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester),	Educational effect number	Way of evaluating educational effect achievement

C – concluding (at semester end)		
F1 (laboratory)	PEK_W01, PEK_U01 – PEK_U03	Assignement 1
F2 (laboratory)	PEK_W02, PEK_U04	Assignement 2
C (laboratory) = 3,0 if (F1 + F2) = 11-12 points. 3,5 if (F1 + F2) = 13-14 points. 4,0 if (F1 + F2) = 15-16 points. 4,5 if (F1 + F2) = 17-18 points. 5,0 if (F1 + F2) = 19-20 points. 5,5 if (F1 + F2) = 19-20 points and F1, F2 were solved using techniques significantly exceeding the course program.		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[3] D. M. Beazley. Programowanie: Python (Wydawnictwo RM, 2002) ISBN: 83-7243-218-X

SECONDARY LITERATURE:

[5] Æ. Frisch. Essential System Administration, Third Edition (O'Reilly, 2002), 3rd edn. ISBN: 978-0596003432.

[6] S. Vugt. Beginning the Linux Command Line (Springer, 2009) ISBN: 978-1-4302-1889-0
http://link.springer.com/book/10.1007/978-1-4302-1890-6/page/1

[7] http://docs.python.org

[8] A. B. Downey. Python for Software Design: How to Think Like a Computer Scientist (Cambridge University Press, 2009), 1st edn. ISBN: 978-0521725965.
http://www.greenteapress.com/thinkpython/index.html

[9] M. Pilgrim. Dive Into Python (Apress, 2004), 1st edn. ISBN: 978-1590593561.
http://www.diveintopython.net

[10] M. L. Hetland, Beginning Python (Springer, 2005) ISBN: 978-1-59059-519-0
http://link.springer.com/book/10.1007/978-1-4302-0072-7/page/1

[11] H. P. Langtangen. A Primer on Scientific Programming with Python (Springer, 2011) ISBN: 978-3-642-18365-2
http://link.springer.com/book/10.1007/978-3-642-18366-9/page/1

[12] K. D. Lee. Python Programming Fundamentals (Springer, 2011) ISBN: 978-1-84996-536-1
http://link.springer.com/book/10.1007/978-1-84996-537-8/page/1

[13] http://docs.scipy.org/doc

[14] http://matplotlib.org/contents.html

[15] http://dev.mysql.com/doc

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Applied informatics

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
PEK_W01	S2Abt5_U05	C2	La4-La12	N1-N4
PEK_W02	S2Abt5_U05	C4	La13-La15	N1-N4
PEK_U02	S2Abt5_U05	C2	La4-La12	N1-N4
PEK_U05	S2Abt5_U05	C4	La13-La15	N1-N4

** - enter symbols for main-field-of-study/specialization educational effects
*** - from table above

Wrocław University of Technology
FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Bioinformatyka**
Name in English	**Bioinformatics**
Main field of study (if applicable)	**Biotechnology**
Specialization (if applicable)	**Bioinformatics**
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**BTC024011**
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)	120				
Form of crediting	exam				
For group of courses mark (X) final course					
Number of ECTS points	4				
including number of ECTS points for practical (P) classes	0				
including number of ECTS points for direct teacher-student contact (BK) classes	1				

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basics of biochemistry and/or molecular biology
2. Basics of programming
3. Basics of molecular modeling
4. Basics of probability theory

SUBJECT OBJECTIVES	
C1	Student knowledge on available sequence, structure and other biology related databases and how to search them efficiently.
C2	Student knowledge on methods of sequence alignment and comparison,

	interpretation of similarity measures and relation between similarity and homology; and applications to sequence similarity based database searches.
C3	Student knowledge on multiple sequence alignment (MSA) calculation methods and applications of MSA to define sequence similarity profiles within families of homologs, to phylogenetic analysis, to secondary and tertiary structure prediction methods, and to function prediction.
C4	Student knowledge on searching for distant homologs using similarity profiles.
C5	Student knowledge on theoretical models of evolution and their limitations, on the definition and evaluation of evolutionary distances between sequences, and on applications of these theoretical models to molecular phylogenetic analysis.
C6	Student knowledge on methods of evaluation of similarity between tertiary structures and structure similarity based database searches.
C7	Student knowledge on sequence based structure prediction methods.
C8	Student knowledge on how to automate database searches and common bioinformatics analyses with the use of specialized programming tools and libraries.
C9	Student knowledge on experimental analysis methods specific to bioinformatics.

SUBJECT EDUCATIONAL EFFECTS

[16] **Relating to knowledge:**

Student who has completed this course knows:

PEK_W01 – databases of biological sequences and structures, databases of metabolic, biochemical, pharmaceutical and medical information; knows where to search for specific information and what tools are available;

PEK_W02 – specific bioinformatics vocabulary, concepts of sequence and structure similarity, definition and types of sequence homology; knows various measures of similarity, how they are calculated and how to interpret their meaning; knows the definitions of evolutionary distance, scoring matrices, similarity profiles and methods of comparisons of tertiary structures;

PEK_W03 – programs for sequence alignments and similarity calculation, programs for similarity based database searches, programs for calculation of multiple sequence alignments and similarity profiles, and programs to compare structural similarity;

PEK_W04 – models of sequence evolution and methods for evaluation of evolutionary distances; knows methods of phylogenetic analysis and has basic knowledge on their effectivity and applicability;

PEK_W05 – selected methods of sequence-based secondary and tertiary structure prediction methods;

PEK_W06 – how to apply the Python programming language and the specialized Biopython library to automate database searches and analyses of data related to bioinformatics;

PEK_W07 – selected analytical methods used in experimental research related to bioinformatics and their applications.

Relating to skills:

Student who has completed this course can:

PEK_U01 – Interpret sequence similarity measures, especially the E-value, and conclude about homology relations between biomolecular sequences or structures based

on these measures;
PEK_U02 – Compare various methods of phylogenetic analysis;
PEK_U03 – Compare various methods of sequence based structure prediction.

Relating to social competences:
Student who has completed this course can:
PEK_K01 – communicate using the specialized bioinformatics vocabulary.

PROGRAMME CONTENT		
Form of classes - lecture		**Number of hours**
L_1	Biological sequences and databases	2
L_2	Homology and similarity	2
L_3	Optimal measures of similarity	2
L_4	Searching for homology	2
L_5	Multiple sequence alignments	2
L_6	Models of molecular evolution	2
L_7	Phylogenetics	4
L_8	Methods of pattern recognition	2
L_9	Similarity of 3D structures	2
L_10	Structure prediction methods	2
L_11	Programming with Biopython	6
L_12	Analytic techniques in bioinformatics	2
	Total hours	30

TEACHING TOOLS USED	
N1	Informational lecture
N2	Lecture with problem solving
N3	Multimedia presentation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
C	PEK_W01-PEK_W07, PEK_U01-	exam

	PEK_U03, PEK_K01	

Exam score	**Grade**
50-60%	3,0 (sufficient)
61-70%	3,5 (sufficient plus)
71-80%	4,0 (good)
81-90%	4,5 (good plus)
91-100%	5,0 (very good)

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

Selected books available in the local library:

1. S.Q. Ye, Bioinformatics. A practical approach, Chapman & Hall/CRC, 2008
2. I. Eidhammer, I. Johanssen, W.R. Taylor, Protein Bioinformatics - an algorythmic approach to sequence and structure analysis, Wiley 2004
3. P.E. Bourne & H. Weissig (ed.), Structural Bioinformatics, Wiley 2003
4. A.D. Baxevanis, B.F.F. Oullette, Bioinformatics, Wiley, 2001

SECONDARY LITERATURE:

There are lots of valuable resources on the Internet; recommended ones are for example available from the National Center for Biotechnology Information:

[1] http://www.ncbi.nlm.nih.gov/guide/training-tutorials/
[2] http://www.ncbi.nlm.nih.gov/books/
[3] Dokumentacja programów bioinformatycznych (BLAST, Modeller, Rosetta, Phylip, HMMER, etc.)
[4] Publikacje w specjalistycznych czasopismach bioinformatycznych

SUBJECT SUPERVISOR
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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Bioinformatics.

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology.

SPECIALITY:

Bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives ***	Programme content***	Teaching tool number ***
(knowledge) PEK_W01	S2Abt5_W03, T2A_W03, T2A_W07, InzA_W02	C1	L_1	N1
PEK_W02		C2	L_2, L_3, L_9	N1, N2
PEK_W03		C3	L_3, L_4	N1
PEK_W04		C5	L_5, L_6, L_7	N1, N2
PEK_W05		C7	L_10	N1
PEK_W06		C8	L_11	N2
PEK_W07		C9	L_12	N1, N3
(skills) PEK_U01	S2Abt5_U04, T2A_U01, T2A_U07	C2	L_2, L_3	N2
PEK_U02		C5	L_7	N1, N2
PEK_U03		C7	L_10	N1
(social competences) PEK_K01		C1-C9	L_1-L_12	N1

** - enter symbols for main-field-of-study/specialization educational effects
*** - from table above

Wrocław University of Technology
FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Bioinformatyka**
Name in English	**Bioinformatics**
Main field of study (if applicable)	**Biotechnology**
Specialization (if applicable)	**Bioinformatics**
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**BTC024011**
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

5. Basics of biochemistry and/or molecular biology
6. Basics of programming and computer usage skills
7. Basics of molecular modeling methods
8. Basics of probability theory

SUBJECT OBJECTIVES

The course should teach the following skills:

C1	Efficient mining of sequences, structures and related information from a range of biotechnology related databases based on complex, specific, keyword-based queries and logical operators;

C2	Searching for sequences and structures of homologous proteins and nucleic acids based on evaluation and interpretation of sequence similarity measures and their relation to homology between sequences;
C3	Creation of sequence similarity profiles and they utilization for more sensitive searches for distant homologs;
C4	Calculation, verification and correction of multiple sequence alignments (MSA);
C5	Performing MSA-based molecular phylogenetic analysis and evaluate the reliability of the results using bootstrap statistical evaluation method;
C6	Use specialized software to create models of tertiary protein structures based on sequence;
C7	Ability to utilize the Python programming language and the Biopython library to fetch and process bioinformatics data or to support and automate analysis tasks.

SUBJECT EDUCATIONAL EFFECTS

[17] **Relating to knowledge:**

[18] Student who has completed this course knows:

PEK_W01 – databases of biological sequences and structures, databases of metabolic, biochemical, pharmaceutical and medical information; knows where to search for specific information and how to buid queries;

PEK_W02 – selected measures of similarity and methods and programs for pairwise sequence alignment and comparison;

PEK_W03 – selected methods and programs for calculation of multiple sequence alignments (MSA); knows applications of MSA's to calculate similarity profiles, to recognize functional elements and to predict secondary and tertiary structures by homology.

PEK_W04 – basic methods and selected programs for sequence based structure prediction.

Relating to skills:

Student who has completed this course can:

PEK_U01 – effectively create complex, specific queries to retrieve only the relevant information or biological sequences from a selection of databases; complete information from multiple sources.

PEK_U02 – search for homologous sequences and structures of biomolecules by sequence similarity and correctly interpret homologs based on evaluation of similarity. Can utilize sequence similarity profiles for identification of distant homologs with low sequence similarity.

PEK_U03 – use selected programs to calculate alignments of multiple sequences, visualize them, verify the proper alignment of conservative residues and introduce corrections where necessary.

PEK_U04 – perform MSA-based molecular phylogenetic analysis, and evaluate the reliability of results using statistical bootstrap analysis.

PEK_U05 – utilize selected software to predict protein structure based on sequence, to evaluate the quality of modela and to compare similarity of related tertiary structures.

PEK_U06 – write his own programs using the Python language and the Bioinformatics library to fetch and process data from databases, convert formats, and support or automate other tasks.

PROGRAMME CONTENT		
Form of classes - laboratory		**Number of hours**
La1	Introductory classes	2
La2	Databases at NCBI, Uniprot, KEGG, Brenda, PDB; query syntax, boolean operators and text based specific searches	4
La3	Similarity based searches for related sequences with BLAST variants. Application of similarity profiles to identification of distant homologs.	4
La4	Examples of problem solving using Python programming with Biopython libraries	2
La5	Calculation, verification and correction of multiple sequence alignments (MSA).	4
La6	Phylogenetic analysis with selected methods	4
La7	Statistical bootstrap analysis of the reliability of the phylogentic analysis	4
La8	Prediction of protein tertiary structure from the sequence	4
La9	Crediting classes	2
	Total hours	30

TEACHING TOOLS USED	
N1	Presentation
N2	Demonstration
N3	Supervised/directed practical problem solving
N4	Individual problem solving
N5	Programming small Python scripts for selected applications, with and without supervision

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1 = 0-5 score points	PEK_W01, PEK_U01	Individual tasks: collection of specific information from multiple databases (1)
F2 = 0-6 score points	PEK_W02, PEK_U02	Individual tasks: search for and evaluation of distant homology based on similarity profiles (2)
F3 = 0-3 score points	PEK_W03, PEK_U03	Individual tasks: calculation, verification and correction of the MSA of a family of

		sequences (3)
F4 = 0-7 score points	PEK_U04	Individual tasks on phylogenetic and bootstrap analysis (4)
F5 = 0-5 score points	PEK_U05	Individual tasks on protein structure prediction (5)
F6 = 0-4 score points	PEK_U06	Utilization of Python and Biopython programming in the tasks (1)-(5)

C = 3,0 for the total score in range 15-17,5
3,5 for the total score in range 18-20,5
4,0 for the total score in range 21-23,5
4,5 for the total score in range 24-26,5
5,0 for the total score in range 27-30

The excellent grade (5,5) can be granted for more extensive use of Biopython or for application of programs and methods not covered during the course.

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

5. Lecture on Bioinformatics
6. Instructions provided for the classes

SECONDARY LITERATURE:

[5] Documentation of the utilized software, available on the relevant WWW pages
[6] Biopython documentation: http://biopython.org
[7] I. Eidhammer, I. Johanssen, W.R. Taylor, Protein Bioinformatics - an algorithmic approach to sequence and structure analysis, Wiley 2004
[8] P.E. Bourne & H. Weissig (ed.), Structural Bioinformatics, Wiley 2003

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Bioinformatics.

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology.

SPECIALITY:

Bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives ***	Programme content***	Teaching tool number ***
(knowledge) PEK_W01	S2Abt5_U04, T2A_U01 T2A_U07	C1	La1, La2	N1
PEK_W02		C2	La3	N1
PEK_W03		C3,C4	La5	N1
PEK_W04		C6	La8	N1
(skills)PEK_U 01		C1	La2	N2, N3, N4
PEK_U02		C2, C3	La3	N2, N3, N4
PEK_U03		C4	La5	N2, N3, N4
PEK_U04		C5	La6, La7	N2, N3, N4
PEK_U05		C6	La4, La8	N2, N3, N4
PEK_U06		C7	La4	N5

** - enter symbols for main-field-of-study/specialization educational effects
*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Bionanotechnologia**
Name in English	**Bionanotechnology**
Main field of study (if applicable)	**biotechnology**
Specialization (if applicable)	**bioinformatics**
Level and form of studies:	**~~1st~~/ 2nd* level, full-time / ~~part-time~~***
Kind of subject	**obligatory / ~~optional / university-wide~~***
Subject code	**BTC024004**
Group of courses	**~~YES~~ / NO***

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30				15
Number of hours of total student workload (CNPS)	90				15
Form of crediting	Examination				crediting with grade
For group of courses mark (X) final course					
Number of ECTS points	3				1
including number of ECTS points for practical (P) classes					1
including number of ECTS points for direct teacher-	1				0.5

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

[1] Basic knowledge of physical chemistry (1st level)

[2] Basic knowledge of biochemistry (1st level)

SUBJECT OBJECTIVES	
C1	Principles underlying the functioning of molecular machines in biology
C2	Basic knowledge about methods utilized in bionanotechnology to design, synthesize and analyze bionanomachines
C3	Practical knowledge on how to perform basic molecular dynamics (MD) simulations to solve problems in bionanotechnology
C4	Basic knowledge on the recent achievements in bionanotechnology

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEK_W01 – Basic concepts of nanobiotechnology and bionanotechnology

PEK_W02 – Principles of functioning of molecular machines in biology

PEK_W03 – Basic knowledge on experimental methods used in design, synthesis and analysis in bionanotechnology

PEK_W04 – Basic knowledge on experimental methods used in structural investigation in bionanotechnology

PEK_W05 – Basic techniques in designing synthetic bionanomachines

PEK_W06 – Basic principles of functioning of bionanomachines

PEK_W07 – Basic knowledge on molecular modelling tools used in designing bionanomachines

Relating to skills:

PEK_U01 – Practical knowledge on how to prepare input files and how to perform minimization and MD of nanopore

PEK_U02 – Practical knowledge of performing basic MD simulations of DNA within the nanopore

PEK_U03 – Practical knowledge on how to prepare and present a seminar on the last achievements in bionanotechnology

PROGRAMME CONTENT		
Form of classes - lecture		Number of hours
Lec 1	**Basic concepts.** Nonotechnology, biotechnology, bionanotechnology, nanobiotechnology. Feynman's idea. Top-down and bottom-up appoaches. Milestone achievements in bionanotechnology. Nanobiotechnology/bionanotechnology in electronics, informatics, energetics, army, agriculture and food technology – examples.	2
Lec 2	**How do molecular machines work in biology?:**Properties of particles at macro- and nano-levels. Bionanomolecules in water environment – hydrophobic effect. Proteins as a structural material in bionanotechnology. Limitations of natural bionanomolecules.	2
Lec 3	**Methods in bionanotechnology: to design, synthesize and analyze.** Rekombinant DNA technology. DNA clonning. PCR method. Protein synthesis in vitro. Directed mutagenesis. Fusion and chimeric proteins. Monoclonal antibodies.	2
Lec 4	**Methods in bionanotechnology: to design, synthesize and analyze – part 2 .** X-ray and NMR methods to investigate structure of biomolecules. Electron spectroscopy methods: TEM, SEM, tomography. AFM method. Molecular modelling as a tool to obtain information on structure and dynamics of biomolecule.	2
Lec 5	**Design of nanomachines.** Methods used in bionanomachines design: sequential covalent bond formation, polimeryzation, self-organizatoin and aggregation. Protein folding. Role of chaperones in folding. Proteins stable in high temperatures. How to make a protein more rigid? How to introduce a disorder in a protein? Symmetric	2

	and quasi-symmetric complexes.	
Lec 6	**Functional aspects of biomoleculs**. Energy transfer in natural bionanomachines. Electron transfer in natural bionanomachines. Light-driven molecular bionanomachines. Charge transfer in biosystems. How do enzymes work? Methods to control bionanomachines – allosteric regulation and covalent modyfication.	2
Lec 7	**Design of bionanomachines.** De novo protein design. Enzyme design based on molecular modelling methods. Design of biosystems having specific spectral properties. PNA (Peptide Nucleic Acid) vs. DNA.	2
Lec 8	**DNA sequencing using MD – part 1**. Construction of a cystal membrane of Si_3N_4. Synthetic nanopore in Si_3N_4.membrane.	2
Lec 9	**DNA sequencing using MD – part 2**. Calibration of force field to reproduce experimental value of dielectric constant.	2
Lec 10	**DNA sequencing using MD – part 3**. Solvation of a nanopore.	2
Lec 11	**DNA sequencing using MD – part 4**. Energy minimization. Molecular dynamics under constant pressure. Measuring ionic current in nanopores.	2
Lec 12	**DNA sequencing using MD – part 5**. Simulating the process of DNA transport through a nonopore.	2
Lec 13	**DNA sequencing using MD – part 6**. Ionic current in nanopores in the presence of DNA. Comparison of ionic current with/without DNA in the system.	2
Lec 14	**DNA sequencing using MD – part 7**. Transporting DNA through nanopore – MD simulation. Transporting ubiquitin through nanopore – MD simulation.	2
Lec 15	**Exam.**	2
	Total hours	

Form of classes - seminar		Number of hours
Sem 1-15	Students in the form of oral contribution present and discuss the late achievements and trends in bionanotechnology based on the most recent scientific literature. The list of possible topics is upgraded every year due to the very rapid progress in this field.	15
	Total hours	**15**

TEACHING TOOLS USED	
N1	Lecture with multimedia presentation
N2	Practical usage of software
N3	Preparation of reports
N4	Seminar presentation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1 (lecture)	PEK_W01 – PEK_W06	Written exam
F2 (lecture)	PEK_W07	Report
P (seminar)	PEK_U01 – PEK_U04	Seminar presentation
P (lecture) = 3.0 if (F1 + F2) = 50-60% max. no of poins. **3.5 if (F1 + F2) = 61-70% max. no of poins.** **4.0 if (F1 + F2) = 71-80% max. no of poins.** **4.5 if (F1 + F2) = 81-90% max. no of poins.** **5.0 if (F1 + F2) = 91-99% max. no of poins.** **5.5 if (F1 + F2) = 100% max. no of poins.**		

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE: [1] E. Gazit "Plenty of room for biology at the bottom: An introduction to bionanotechnology", Imperial College Press, 2007. **SECONDARY LITERATURE:** [1] *Bionanotechnology*: *Proteins to Nanodevices,* Eds. V. Renugopalakrishnan, R.V.Lewis, Springer, 2006. [2] *Nanobiotechnology: Concepts, Applications and Perspectives*, Eds. C.M.Niemeyer, C.A.Mirkin, Wiley-VCH, 2004. [3] *Nanobiotechnology II: More Concepts and Applications*, Eds. C.M.Niemeyer, C.A.Mirkin, Wiley-VCH, 2007.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
dr hab. Tadeusz Andruniów, tadeusz.andruniów@pwr.wroc.pl

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Bionanotechnology.

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Bionanotechnology, specialization: Bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**	S2bt5_W07	C1	Wy1	N1
PEK_W02	S2bt5_W07	C1	Wy2	N1

PEK_W03	S2bt5_W07	C2	Wy3	N1
PEK_W04	S2bt5_W07	C2	Wy4	N1
PEK_W05	S2bt5_W07	C2	Wy5	N1
PEK_W06	S2bt5_W07	C1	Wy6	N1
PEK_W07	S2bt5_W07	C3	Wy7-Wy14	N1, N2, N3
(skills) **PEK_U01**	S2bt5_U10	C4	Wy8– Wy10	N2
PEK_U02	S2bt5_U10	C4	Wy11 – Wy14	N2, N3
PEK_U03	S2bt5_U10	C4	Se1-Se8	N4

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Projekt bioprocesowy**
Name in English	**Bioprocess project**
Main field of study (if applicable)	**Biotechnology**
Specialization (if applicable)	**Bioinformatics**
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**BTC024015**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)				30	
Number of hours of total student workload (CNPS)				90	
Form of crediting				crediting with grade	
For group of courses mark (X) final course					
Number of ECTS points				3	
including number of ECTS points for practical (P) classes				3	
including number of ECTS points for direct teacher-				3	

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[19] Mathematics [20] Physics [21] Physical chemistry

SUBJECT OBJECTIVES	
C1	Understanding and practical implementation of the knowledge about designing of biotechnological unit processes
C2	Working knowledge of using a basic commercial software for designing of processes, calculation of optimal process parameters, making up material and energy balances, and estimating costs of processing
C3	Familiarization with the practical examples of computation, design, and optimization of unit operations in biotechnological processes

SUBJECT EDUCATIONAL EFFECTS

Relating to skills:

PEK_U01 – understands and can apply the design principales within the thermodynamics, equilibrium and kinetics of unit operations.

PEK_U02 – can use the professional software to calculate the optimal parameters of bioprocess.

PEK_U03 – is able to select and design the production and separation of bioproduct procedures and the order of unit operations.

PEK_U04 – can identify the bottlenecks of bioprocess.

PEK_U05 – has the working knowledge of using a professional software to evaluate the economics of the bioprocess.

PEK_U06 – can discuss the exemplary bioprocesses within the environment protection, and bioproducts production and separation.

PROGRAMME CONTENT		
Form of classes - project		Number of hours
Proj 1	Organising class. Familiarisation with the safety rules in the computer room. Teaching tools and conditions of course credition. Classification and applications of unit processes in biotechnology.	2
Proj 2	Basic principles in designing of biotechnological processes: conservation laws, thermodynamical laws, equilibrium, and kinetics of unit processes. Material and energy balances.	2
Proj 3	Formulation and analysis of the problem, exemplary solutions, additional methods and techniques. Introduction to SuperPro Designer software: user interface, database.	2
Proj 4	Determination of optimal process parameters, conditions, and layout.	2
Proj 5	Mixing in designing od biotechnological processes.	2
Proj 6	Designing of diffusional processes of separation: distillation, extraction, absorption, chromatography, adsorption, crystallization and drying.	2
Proj 7	Designing of heat exchangers.	2
Proj 8	Designing of membrane processes for recovery, purification and concentration of bioproducts.	2
Proj 9	Scheduling. Gantt chart.	2
Proj 10	Bottlenecks of the process.	2
Proj 11	Economic evaluation of biotechnological processes. Cost calculations. Energy consumption and equipment size. Scaling-up.	2
Proj 12	Design of biotechnological processes considering environmental impact.	2
Proj 13	Exemplary processes of industrial and municipial wastewater treatment, and water purification.	2
Proj 14	Exemplary processes of production and separation of bioproducts.	2
Proj 15	Presentation of the final project. Course acceptance.	2
	Total hours	**30**

TEACHING TOOLS USED	
N1	Multimedia presentations
N2	Solving the exemplary issues during the classes
N3	Using of the commercial software

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1-F3	PEK_U01-PEK_U05	partial projects made in a professional software
F4	PEK_U01-PEK_U05	final project made in a professional software
C=0,4(F1+F2+F3)/3+0,6F4		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] E. Heinzle, A.P. Biwer, C.L. Cooney - Development of Sustainable Bioprocesses: Modeling and Assessment, Viley 2006 (PWr. On-line library).

SECONDARY LITERATURE:

[1] R.G. Harrison, P. Todd, S.R. Rudge, D.P. Petrides - Bioseparations Science and Engineering, Oxford 2002.
[2] M.C. Flickinger - Encyclopedia of Industrial Biotechnology, Bioprocess, Bioseparation, and Cell Technology, Volumes 1-7, John Wiley & Sons, 2010.

SUBJECT SUPERVISOR

(NAME AND SURNAME, E-MAIL ADDRESS)

Dr inż. Izabela Polowczyk, izabela.polowczyk@pwr.wroc.pl

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Bioprocess project

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology

AND SPECIALIZATION

Bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(umiejętności) PEK_U01	S2Abt5_U13	C1	Proj1-Proj3	N1, N2
PEK_U02	S2Abt5_U13	C1, C2	Proj4	N1, N2, N3
PEK_U03	S2Abt5_U13	C1, C2	Proj5-Proj9	N1, N2, N3
PEK_U04	S2Abt5_U13	C1, C2	Proj10	N1, N2, N3
PEK_U05	S2Abt5_U13	C1, C2	Proj11	N1, N2, N3
PEK_U06	S2Abt5_U13	C1, C3	Proj12-Proj14	N1, N2

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Praca dyplomowa I**
Name in English	**Graduate laboratory I**
Main field of study (if applicable)	**all fields of study at Faculty of Chemistry**
Specialization (if applicable)	
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**CHC030004**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)			60		
Number of hours of total student workload (CNPS)			120		
Form of crediting			crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points			4		
including number of ECTS points for practical (P) classes			4		
including number of ECTS points for direct teacher-			2		

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[22] Theoretical and practical knowledge required for the degree program being studied [23]

SUBJECT OBJECTIVES	
C1	Get to know the basic methodology of scientific work
C2	Acquisition of the ability to use the scientific literature and other sources of knowledge.
C3	Increasing knowledge in a specialized field being studied

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

Student:

PEK_W01 – knows the types of sources of scientific knowledge and expertise,

PEK_W02 - has in-depth knowledge in the area of the thesis topics.

Student:

Relating to skills:

PEK_U01 – able to collect and verify the information useful to know a particular issue,

PEK_U02 – can combine and generalize information from different sources,

PEK_U03 – able in a concise and critical to develop the information collected,

PROGRAMME CONTENT

Form of classes - laboratory		Number of hours
La 1-15	Individual student's work according to the schedule agreed with the thesis supervisor.	60
	Total hours	**60**

TEACHING TOOLS USED	
N1	consultations

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
C	PEK_W01 PEK_W02 PEK_U01 – PEK_U03	evaluation of the quantity and quality of student work

PRIMARY AND SECONDARY LITERATURE
[1] The scientific and professional literature designated by the Supervisor and / or found by the student.

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

Card preparation: **Piotr Drożdżewski,** piotr.drozdzewski@pwr.wroc.pl

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Graduate laboratory I

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

(all fields of study)

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**	K2Abt_U02**,** K2Ach_U05, K2Aic_U02, K2Aim_U06, K2Atc_U09	C2	La1-La15	N1
PEK_W02	K2Abt_U02**,** K2Ach_U05, K2Aic_U02, K2Aim_U06, K2Atc_U09	C4	La1-La15	N1
(skills) **PEK_U01**	K2Abt_U02**,** K2Ach_U05, K2Aic_U02, K2Aim_U06, K2Atc_U09	C1, C2	La1-La15	N1
PEK_U02	K2Abt_U02**,** K2Ach_U05, K2Aic_U02, K2Aim_U06, K2Atc_U09	C1, C3	La1-La15	N1
PEK_U03	K2Abt_U02**,** K2Ach_U05, K2Aic_U02, K2Aim_U06, K2Atc_U09	C1, C3	La1-La15	N1

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Praca dyplomowa II**
Name in English	**Graduate laboratory II**
Main field of study (if applicable)	**all fields of study at Faculty of Chemistry**
Specialization (if applicable)	
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**CHC030005**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)			225		
Number of hours of total student workload (CNPS)			300		
Form of crediting			crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points			10		
including number of ECTS points for practical (P) classes			10		
including number of ECTS points for direct teacher-			7,5		

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[24] Theoretical and practical knowledge required for the degree program being studied [25]

SUBJECT OBJECTIVES	
C1	Get to know the basic methodology of scientific work
C2	Gaining the skills of planning, carrying out and analyzing the results of scientific experiments
C3	Increasing knowledge in a specialized field being studied
C4	Inspiring students to their further development and continuous self-education.
C5	Deepening the ability to create a written document presenting the current state of knowledge and their own achievements in the field of thesis topic.

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

Students:

PEK_W01 – knows the types of sources of scientific knowledge and expertise,

PEK_W02 - has theoretical and practical knowledge necessary to perform the thesis

Students:

Relating to skills:

PEK_U01 – able to carry out experiments / perform project / build software and develop the results and draw conclusions from their achievements,

PEK_U02 – able to prepare a written paper on a selected scientific topic in and their contribution to this issue

PEK_U03 –can find new and develop their existing interests and skills.

PROGRAMME CONTENT

Form of classes - laboratory		Number of hours
La 1-15	Individual student's work according to the schedule agreed with the thesis supervisor.	60
	Total hours	**60**

TEACHING TOOLS USED	
N1	consultations

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
C	PEK_W01 PEK_W02 PEK_U01 – PEK_U03	evaluation of the quantity and quality of student supervisor after submission of the final written version of the study entitled: Diploma Thesis

PRIMARY AND SECONDARY LITERATURE
[2] The scientific and professional literature designated by the Supervisor and / or found by the student.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
Card preparation: **Piotr Drożdżewski,** piotr.drozdzewski@pwr.wroc.pl

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Graduate laboratory II

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

(all fields of study)

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**	K2Abt_U03**,** K2Ach_U06, K2Aic_U03, K2Aim_U07, K2Atc_U10	C1	La1-La15	N1
PEK_W02	K2Abt_U03**,** K2Ach_U06, K2Aic_U03, K2Aim_U07, K2Atc_U10	C3	La1-La15	N1
(skills) **PEK_U01**	K2Abt_U03**,** K2Ach_U06, K2Aic_U03, K2Aim_U07, K2Atc_U10	C2	La1-La15	N1
PEK_U02	K2Abt_U03**,** K2Ach_U06, K2Aic_U03, K2Aim_U07, K2Atc_U10	C5	La1-La15	N1
PEK_U03	K2Abt_U03**,** K2Ach_U06, K2Aic_U03, K2Aim_U07, K2Atc_U10	C4	La1-La15	N1

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology **FACULTY OF CHEMISTRY** **SUBJECT CARD**	
Name in Polish	**Seminarium dyplomowe** (+ praca dyplomowa + przygotowanie do egzaminu dyplomowego)
Name in English	**Graduation seminar and thesis preparation**
Main field of study (if applicable)	
Specialization (if applicable)	
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**BTC024001**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)					15
Number of hours of total student workload (CNPS)					300
Form of crediting					Crediting with grade
For group of courses mark (X) final course					
Number of ECTS points					10
including number of ECTS points for practical (P) classes					10

including number of ECTS points for direct teacher-student contact (BK) classes					0,5

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[26] Theoretical and practical knowledge required for the degree program being studied
[27]

SUBJECT OBJECTIVES	
C1	Skills of oral presentation of own work results
C2	Skills of written presentation own research results.
C3	Get to know the form of a public discussion with regard to defend own views and ideas.
C4	

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

Student:

PEK_W01 – has in-depth knowledge of the thesis topic.

Student:

Relating to skills:

PEK_U01 – can use specific computer tools to prepare a multimedia presentation

PEK_U02 – can submit their prepared multimedia presentations to the public.

PEK_U03 – able to publicly present the results of own achievements, and to defend them during the public discussion.

PROGRAMME CONTENT

Form of classes - seminar		Number of hours
Sem 1-15	Presentation of multimedia presentation and participate in the discussion	15
	Total hours	**15**

TEACHING TOOLS USED	
N1	consultations
N2	multimedia presentation
N3	oral presentation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
C	PEK_W01 PEK_U01 – PEK_U03	evaluation of oral presentation and activities in the discussions

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE: [2] none **SECONDARY LITERATURE:** [3] none [4]

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
Card preparation: **Piotr Drożdżewski,** piotr.drozdzewski@pwr.wroc.pl

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Graduate seminar.

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

(all fields of study)

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**	K2Abt_U33, K2Ach_U41, K2Aic_U27, K2Aim_U34, K2Atc_U36	C3	Se1-Se15	N1
(skills) **PEK_U01**	K2Abt_U33, K2Ach_U41, K2Aic_U27, K2Aim_U34, K2Atc_U36	C1	Se1-Se15	N2
PEK_U02	K2Abt_U33, K2Ach_U41, K2Aic_U27, K2Aim_U34, K2Atc_U36	C1	Se1-Se15	N2
PEK_U03	K2Abt_U33, K2Ach_U41, K2Aic_U27, K2Aim_U34, K2Atc_U36	C2, C3	Se1-Se15	N1

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Instrumentalna analiza leków**
Name in English	**Instrumental drug analysis**
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	**Medicinal chemistry, Bioinformatics**
Level and form of studies:	**~~1st~~/ 2nd* level, ~~full-time / part-time~~***
Kind of subject	**obligatory~~/ optional / university-wide~~***
Subject code	**CHC024004**
Group of courses	**YES ~~/ NO~~***

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15		30		
Number of hours of total student workload (CNPS)	60		60		
Form of crediting	crediting with grade		crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	2		2		
including number of ECTS points for practical (P) classes			2		

including number of ECTS points for direct teacher-student contact (BK) classes	0.5		1		

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[1] Has a general knowledge about fundamentals in analytical chemistry

SUBJECT OBJECTIVES	
C1	Getting to know experimental techniques and procedures of the sample preparation used in basic instrumental analytical techniques of drug analysis
C2	Acquainting with theoretical basis of working and mesurements of instruments for the drug analysis
C3	Getting to know with methods of the sampling and the sample preparation of pharmaceuticals
C4	Obtaining basic skills related to the use of instruments in drug nalysis
C5	Learning how to perform basic calculations necessary to develop results of analyzes carried out

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

The person who passed the course

PEK_W01 – knows basic concepts related to the drug analysis, stages of the analytical procedure, i.e., the preparation of samples and the analysis of active substances

PEK_W02 – knows parameters characterizing instrumental methods of the analysis and why these methods should be validated

PEK_W03 – knows types of spectroscopic methods of the drug analysis, including atomic and molecular spectrometries

PEK_W04 – knows instrumental methods applied for the assessment of the structure of studied compounds, i.e., IR, NMR, XRD

PEK_W05 – knows methods applied for the chromatographic and electrophoretic

separations of compounds

PEK_W06 – knows basic methods of the sample preparation in the drug analysis

Relating to skills:

The person who passed the course

PEK_U01 – can select and apply the most suitable for the type of the sample and the aim of the analysis the method of the sampling and the sample preparation of pharmaceuticals

PEK_U02 – can choose the right for the type of the sample and the aim of the analysis the measurement method

PEK_U03 – can perform the analysis using apparatus suitable for the type of the analysis and the determined component

PEK_U04 – can perform calculations related to results of analyzes and determinations, assess the accuracy of results and verify measurement errors

PROGRAMME CONTENT		
Form of classes - lecture		Number of hours
Lec 1	Introduction to the drug analysis - basic definitions and concepts, steps of the sample preparation and the analysis of active substances	2
Lec 2	Parameters characterizing instrumental methods of the analysis, the validation of methods and procedures	2
Lec 3	Introduction to spectroscopic methods used in the drug analysis	2
Lec 4	Review of atomic and molecular spectroscopic methods of the analysis of pharmaceuticals	2
Lec 5	Overview of methods used in the drug analysis to determine the chemical structure of substances	2
Lec 6	Overview of chromatographic and electrophoretic separation methods used in the drug analysis	2
Lec 7	Techniques used for the preparation of pharmaceuticals to concentrate, separate and isolate substances	3

	Total hours	**15**

Form of classes - laboratory		Number of hours
Lab 1	Conditions for the completion of the course. The safety in the laboratory	2
Lab 2	Testing properties of the formulation containing magnesium lactate	4
Lab 3	The determination of the active ingredients of the formulation	4
Lab 4	The determination of main metallic components of the formulation and impurities	4
Lab 5	The statistical evaluation of results	4
Lab 6	The application of the powder X-ray diffraction analysis of pharmacruticals	4
Lab 7	The determination of trace elements in Polish herbal pharmaceuticals (1) – the preparation of samples	4
Lab 8	The determination of trace elements in Polish herbal pharmaceuticals (2) the use of atomic absorption spectrometry	4
	Total hours	**30**

TEACHING TOOLS USED	
N1	Informative lectures
N2	Implementation of experiments
N3	Preparation of reports
N4	Consultations

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during	Educational effect number	Way of evaluating educational effect achievement

semester), C – concluding (at semester end)		
C (lecture)	PEK_W01 – PEK_W06	Final examination
C (laboratory)	PEK_U01 – PEK_U04	Arithmetic mean of all marks for reports with results of all analyses and experiments made

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1]. A. Kar, Pharmaceutical Drug Analysis, New Age Internation (P) Ltd. Publishers, New Delhi, 2005

[2] D. G. Watson, Pharmaceutical Analysis, Churchill Livingstone, Edinburgh, 1999

[3] S. AHUJA, Stephen SCYPINSKI, Handbook of Modern Pharmaceutical Analysis, Academic Press, San Diego, 2000

SECONDARY LITERATURE:

[1] R. Kellner, J.-M. Mermet, M. Otto, H. M. Widmer (editors), Analytical Chemistry, Wiley-VCH, Weinheim, 1998

[2] Skoog D.A., West D.M., Holler F.J. (1996). Fundamentals of Analytical Chemistry, Saunders College Publishing

[3] WHO (1991). Guidelines for assessment of herbal medicines. Publications of the World Health Organisation, Geneva

SUBJECT SUPERVISOR

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Dr hab. inż. Paweł Pohl, Prof. PWr, pawel.pohl@pwr.wroc.pl

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Instrumental drug analysis

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology, Chemistry

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01 – PEK_W06**	S2Ach4_W03, S2bt5_W06	C1, C2	Lec 1 – Lec 7	N1
(skills) **PEK_U01**	S2Ach4_U03, S2bt5_U09	C3 – C5	Lab 2 – Lab 8	N2, N3, N4

* - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Prawna ochrona własności intelektualnej i problemy etyczne w biotechnologii**
Name in English	**Intellectual property rights and ethical questions in biotechnology**

Main field of study (if applicable): Biotechnology
Specialization (if applicable): BIOINFORMATICS
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code FLC024002w
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					
including number of ECTS points for direct teacher-student contact (BK) classes	1				

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. No prerequisites

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SUBJECT OBJECTIVES

C1 Gaining basic knowledge on the kinds and systems of intellectual property protection, use and commercialization.
C2 Understanding the role and procedures of intellectual property protection, including industrial property (inventions, designs and marks) as well as copyrights (artistic, scientific, literary works, computer programs and databases).
C3 Understanding the legal and economic aspects of intellectual property protection and its use as well as ethical questions and problems connected with biotechnological inventions.
C4 Getting to know different patent (and other IPR) information sources, as well as methods of their use for knowledge protection in innovation processes in biotechnology.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEK_W01Student knows and understands the basic concepts and regulations concerning the IPR protection and commercialization.

PEK_W02 Student has basic knowledge of different types of protectable knowledge and legal systems and procedures of IPR protection in PL, EU, and in the world.

PEK_W03 Student understands the role and value of intellectual property, knows the procedural costs of knowledge protection as well as potential benefits derived from it. Student is also aware of risks connected with IPR infringement cases as well as of risks and controversies connected with ethical aspects and problems in biotechnology field.

PEK_W04 Student has general knowledge of available patent information sources and its use in innovation processes in biotechnology.

PROGRAMME CONTENT

	Form of classes - lecture	**Number**
Lec 1	Introduction. The concept and role of intellectual property protection for modern organizations and in everyday life. Intellectual property protection systems and forms in PL, EU and in the world.	2
Lec 2	Industrial property law – types of protected knowledge, the concept of invention and patent, patentability requirements, patent procedures(PL,EU,WO)	2
Lec 3,4	Specifics of biotech patenting - patent protection for biotechnological inventions and exclusions for ethical reasons, current legislation (Biotech Patent Directive – controversies), development and implications of patent law in the field of biotechnology and genetic engineering, history and statistics of biotech patenting, controversial biotech patents - examples.	4
Lec 5	Patenting trends in the world.	2
Lec 6	Trademarks – definition and protection procedures and requirements. Geographical indications protection systems.	2
Lec 7	Utility Models, Designs and know-how – definitions and protection systems	2
Lec 8	The use of available patent information databases – examples and practical searches of protected knowledge in biotechnology. Biotechnological patent searching excersises.	2
Lec 9,10	Copyrights and related rights – creative and scientific works protection, software and database protection, subject, object and time of protection	4
Lec 11,12	IPR infringement cases in biotechnology, IPR limitations, ethical aspects of IPR protection, pros and cons of different types of protection, use and commercialization of IPRs, freedom to operate.	4
Lec	Convention on Biological Diversity, Traditional Knowledge and Genetic	2

13	resources protection and benefit sharing, International Treaty on Plant Genetic Resources for Food and Agriculture. Discussing the future of biotech patenting	
Lec 14	Discussion on ethical aspects of biotech patenting and Opinions of the Commission's European Group on Ethics in Science and New Technologies	2
Lec 15	Test	2
	Total hours	30

TEACHING TOOLS USED

N1. Lecture with multimedia presentations
N2. Internet patent information databases searches

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1	PEK_W01 –W04	Written report with completed tasks
F2	PEK_W01 –W04	Activity, presence
P = 0,6*F1 + 0,4*F2		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

1. L. Bently, B. Sherman, *Intellectual Property Law*, Oxford University Press, 2008.
2. Ed. by D. Castle, *The Role of Intellectual Property Rights in Biotechnology Innovation*, Edward Edgar, 2009.
3. Ed. by E. Arezzo, G. Ghidini, *Biotechnology and Software Patent Law*, Edward Edgar, 2011.

SECONDARY LITERATURE:

Internet sites: www.uprp.pl, www.epo.org, www.wipo.org, uspto.org, OHIM, etc.

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

Lidia Żurawowicz, lidia.zurawowicz@pwr.wroc.pl

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT
Intellectual Property Rights and ethical questions in biotechnology
AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY
Biotechnology
AND SPECIALIZATION Bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
PEK_W01 (knowledge)	K2Abt_W05	C1- C2	Lec1-Lec14	N1, N2

** - enter symbols for main-field-of-study/specialization educational effects
*** - from table above

Faculty of Chemistry

Course card

Course name in Polish **Wstęp do statystyki praktycznej**

Name in English **Introduction to the practical statistics**

Major (if applicable) Biotechnology

Specialization (if applicable): Bioinformatics

Level and form of studies: **II level*, full-time / ~~part time*~~**

Kind of course: **obligatory~~/ optional / university-wide*~~**

Course code **MAP003047**

Group of courses **-YES / ~~NO~~***

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15	15			
Number of hours of total student workload (CNPS)	60	30			
Form of crediting	Examination / ~~crediting with grade~~*	Examination ~~/ crediting with grade*~~	Examination / crediting with grade*	Examination / crediting with grade*	Examination / crediting with grade*
For group of courses mark (X) final course					
Number of ECTS points	2	1			
including number of ECTS points for practical (P) classes		1			
including number of ECTS points for direct	0,5	0,5			

teacher-student contact (BK) classes					

*delete if not applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

7. Student has understands and applies basic notions of mathematical analysis..
8. Student knows probability theoryas required on matura at basic level.

COURSE OBJECTIVES

C1 Learn descriptive statistics and visualization of data.

C2 Learn basic notions of probability and their applications in mathematical 55odeling.

C3 Learn to build statistical models and formulate necessary assumptions.

C4 Learn to select procedures to given statistical analyses.

*delete if not applicable

1. Course educational effects

Concerning knowledge, student knows:

PEK_W01 basic graphical methods of presenting data and procedures leading to them

PEK_W02 how to model random phenomena and apply probability models

PEK_W03 basic descriptive statistics and their numerical procedures

PEK_W04 methods of estimation for basic parametric models

PEK_W05 tests of significance for parameters in parametric models and basic non-parametric models

Concerning skills, student can:

PEK_U01 apply basic graphical methods to present experimental data

PEK_U02 perform basic calculations related to probability models

PEK_U03 select and calculate descriptive statistics to experimental data and calculate them

PEK_U04 select statistical test to analyze typical experimental data

Concerning social skills, student:

PEK_K01 is able to find knowledge in the bibliography of the course

PEK_K02 is able to use software for basic analysis of statistical models

PEK_K03 understands the need for systematic own work to master the course's material

COURSE CONTENT		
2. Form of classes – lecture		**1. Number of hours**
Wy1	Visual and numerical description of data. Variables. Frequency histogram. Typical statistics: mean, median, quantiles, variance, standard deviation. Linear transformations of variables. Densities. Skewness. Normal distribution: probabilities and quantiles. Standardization. Normal probability plot.	2
Wy2	Explanatory and response variables. Scatterplot. Linear regression. Correlation. Residuals. Causality. Experimental and observational studies. Controls. Sampling and randomization. Random numbers. Block designs. Statistical significance. Parameters and statistics. Sampling distributions. Bias and variability.	2
Wy3	Binomial distribution in sampling: probabilities and parameters. Means and sums in the binomial setting. Central limit theorem for the binomial distribution. Sampling distribution of the sample mean: their expectation and standard deviation. Independence. Central limit theorem for the sample mean.	2
Wy4	Tests of significance. Tests for the mean based on the central limit theorem. Hypotheses, P-value, significance level, directional and non-directional tests. Statistical significance and practical importance. Bonferroni correction.	2
Wy5	Significance tests and confidence intervals based on Student distribution. One-sample and two-samples tests. Significance tests and confidence intervals for proportions. Planning the size of the experiment.	2

Wy6	Contingency tables. Joints, marginal and conditional distributions. Chi-square test for independence. Simpson paradox. Statistical models for linear regression. Confidence intervals for parameters and prediction in regression.	2
Wy7	Analysis of variance. Structure of data. Hypotheses and test statistics. Pairwise comparisons.	2
Wy8	Final	1
	Total hours	**15**

Form of classes – recitation		**Number of hours**
Ćw1	Describing distributions. Calculating basic statistics. Calculations for the normal distributions.	2
Ćw2	Planing and performing statistical studies.	2
Ćw3	Calculating sampling distributions and their parameters. Approximate normal calculations.	2
Ćw4	Formulating hypotheses, calculating P-values, performing normal tests.	2
Ćw5	Midterm	1
Ćw6	T-tests and confidence intervals for means. Tests and intervals for proportions. Plan sufficient sample size.	2
Ćw7	Test for independence in contingency tables.	2
Ćw8	Perform statistical analysis of linear regression and one-factor analysis of variance.	2
	Total hours	**15**

3. TEACHING TOOLS USED

N1. Lecture – traditional method

N2. Classes – traditional method (*exercises solving and discussion)*

N3. Office hours N4. Student's own work – preparation for the classes

EVALUATION OFCOURSE'S EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
P-Wy	PEK_W01-PEK_W05 PEK_K01-PEK_K03	test
P-Ćw	PEK_U01-PEK_U04 PEK_K01-PEK_K03	oral presentations, quizzes, test
P=1/2*Wy+1/2Ćw		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

9. J. Koronacki, J. Mielniczuk, Statystyka dla studentów kierunków technicznych i przyrodniczych, WNT, Warszawa 2004.
10. L. Gajek, M. Kałuszka, Wnioskowanie statystyczne. Modele i metody. WNT, Warszawa 2004.
11. J. Greń, Statystyka matematyczna. Modele i zadania, PWN, Warszawa 1976.
12. W. Kordecki, Rachunek prawdopodobieństwa i statystyka matematyczna. Definicje, twierdzenia, wzory, Oficyna Wydawnicza GiS, Wrocław 2002.
13. H. Jasiulewicz, W. Kordecki, Rachunek prawdopodobieństwa i statystyka matematyczna. Przykłady i zadania. GiS, Wrocław 2001.

SECONDARY LITERATURE:

[9] T. Inglot, T. Ledwina, Z. Ławniczak, Materiały do ćwiczeń z rachunku prawdopodobieństwa i statystyki matematycznej, Wydawnictwo Politechniki Wrocławskiej, Wrocław 1984.

[10] W. Klonecki, Statystyka matematyczna, PWN, Warszawa 1999.

[11] W. Krysicki, J. Bartos, W. Dyczka, K. Królikowska, M. Wasilewski, Rachunek prawdopodobieństwa i statystyka matematyczna w zadaniach, Cz. I-II, PWN,

Warszawa 2007.
[12] D. Moore, G. McCabe, Introduction to the Practice of Statistics, ed. IV, Freeman, 2003.

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

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Komisja programowa Instytutu Matematyki i Informatyki

MATRIX OF CONNECTIONS BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Introduction to the practice of statistics

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY **……**
AND SPECIALIZATION …..

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
PEK_W01 (knowledge)		C1, C2	Wy1	1,3,4
PEK_W02		C1-C4	Wy1-Wy8	1,3,4
PEK_W03		C1	Wy4-Wy8	1,3,4
PEK_W04		C1, C3, C4	Wy4, Wy5	1,3,4
PEK_W05		C1, C3, C4	Wy6-Wy8	1,3,4
PEK_U01 (skills)		C1	Ćw1, Ćw8	1,2,3,4
PEK_U02		C1-C4	Ćw1-Ćw4, Ćw8	1,2,3,4
PEK_U03		C1	Ćw5, Ćw8	1,2,3,4
PEK_U04		C1, C3, C4	Ćw6-Ćw8	1,2,3,4
PEK_K01 (competences)		C1-C4	Wy1-Wy8 Ćw1-Ćw8	1,2,3,4
PEK_K02		C1-C4	Wy1-Wy8 Ćw1-Ćw8	1,2,3,4
PEK_K03		C1-C4	Wy1-Wy8 Ćw1-Ćw8	1,2,3,4

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

FACULTY OF CHEMISTRY / DEPARTMENT OF CHEMICAL AND BIOCHEMICAL PROCESSED

SUBJECT CARD

Name in Polish:	Metody matematyczne w projektowaniu i analizie eksperymentu
Name in English	**Mathematical methods in the design and analysis of the experiment**
Main field of study (if applicable):	**Biotechnology, Chemistry, Materials Science, Chemical Technology**
Specialization (if applicable):	
Level and form of studies:	**2nd level, full-time**
Kind of subject:	**obligatory**
Subject code:	**MAC024001**
Group of courses:	**Yes**

*delete if not related

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15				
Number of hours of total student workload (CNPS)	30				
Form of crediting	Credited with grade				
For group of courses mark (X) final course					
Number of ECTS points	1				
including number of ECTS points for practical (P) classes					
including number of ECTS points for direct teacher-student contact (BK) classes	0,5				

* delete if not related

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Completion of Calculus I, Algebra I
2. Ability to use computer.

SUBJECT OBJECTIVES	
C1	To understand application of statistical modeling in chemical experiment.
C2	To learn application of numerical implementation of statistical and optimization methods in control of chemical process.
C3	To understand mathematical apparatus of various problems related with design and analysis of the experiment.
C4	To learn how to process experimental data using statistical using numerical packages.

SUBJECT EDUCATIONAL EFFECTS

The range of skills:
The person who completed the course:
PEK_W01 – is able to process experimental data and empirical observations and understand the role of statistical and mathematical methods in its description,
PEK_W02 - is able to relate physical and chemical problem with appropriate mathematical problem and method to solve it
PEK_W03 – has a scope of knowledge of mathematics and computer science to describe and interpret natural phenomena is able to process them using mathematical and statistical methods, is able to calculate a level of correlation between data and fit appropriate model, is able to solve set of linear, nonlinear and differential equations,
PEK_W04 – using appropriate numerical method and numerical packages MATLAB, Excel and Origin is able to solve given mathematical problem with given accuracy

With a range of social skills:
The person who completed the course:
PEK_K01 – understand the need of self-education using appropriate scientific and technical literature.

PROGRAMME CONTENT		
Form of classes - laboratory		**Number of hours**
Le1	Solving sets of linear equations, matrix equations, inverse matrix, Gauss algorithm: case studies using MATLAB.	2
Le2	Solving sets of nonlinear equations, solution location, Newton-	2

	Raphson method: case study using MATLAB.	
Le3	Solving sets differentials equations, Euler method, Verlet method, explicit and implicit scheme: case study using MATLAB	2
Le4	Linear regression – least squares method, correlation coefficient, sum of squares, error: case study using MATLAB and Excel	2
Le5	Nonlinear regression, linearization, normal equation, Gauss-Newton method: case study using MATAB and Excel.	2
Le6	Fitting model, chi-square test, Kolmogorov-Smirnov test, Grubb test: case study using Origin and MATLAB.	2
Le7	Statistical hypothesis testing, normal distribution, t-Student distribution, ANOVA: case study using Origin and Excel.	2
Le8	Response surface method, Box-Benhken method: case study using MATLAB.	1
	Total hours	15

TEACHING TOOLS USED	
N1	Presentation.
N2	Computer presentation.
N3	Student's self study.
N4	Consultation.

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
P	K1Aic_U08, K1Aic_U11, K1Aic_U19, K1Aic_U25	Test.
grade	**2,0** if P < 25 pnt. **3,0** if P= 25,5– 28 pnt. **3,5** if P = 28,5 – 31 pnt. **4,0** if P = 31,5 – 34 pnt. **4,5** if P = 34,5- 37 pnt. **5,0** if P = 40 - 45 pnt. **5,5** if P = 45,5- 50 pnt.	

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE [1] Steven C. Chapra, Applied Numerical Methods with MATLAB: for Engineers and Scientists, McGrew 2012 **SECONDARY LITERATURE:** Internet sources.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
Dr inż. Łukasz Radosiński **Lukasz.radosinski@pwr.wroc.pl**

MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT
Mathematical methods in the design and analysis of the experiment.
AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) PEK_W01	K2Abt_W01, K2Ach_W01, K2Aic_W01, K2Aim_W01, K2Atc_W01	C1-C4	Le1-Le8	N1-N4
PEK_W02	K2Abt_W01, K2Ach_W01, K2Aic_W01, K2Aim_W01, K2Atc_W01	C1-C3	Le1-Le8	N1-N4
PEK_W03	K2Abt_W01, K2Ach_W01, K2Aic_W01, K2Aim_W01, K2Atc_W01	C1, C3, C4	Le1-Le8	N1-N4
PEK_W04	K2Abt_W01, K2Ach_W01, K2Aic_W01, K2Aim_W01, K2Atc_W01	C2, C4	Le1-Le8	N1-N4
(social skills) PEK_K01	K2Abt_W01, K2Ach_W01, K2Aic_W01, K2Aim_W01, K2Atc_W01	C1-C4	Le1-Le8	N1-N4

** - enter symbols for main-field-of-study/specialization educational effects
*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Metodologia badań doświadczalnych**
Name in English	**Methodology of experimental research**
Main field of study (if applicable)	**Biotechnology**
Specialization (if applicable)	**Bioinformatics**
Level and form of studies:	**1st level, full-time**
Kind of subject	**obligatory**
Subject code	**FLC024003**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	2				
Number of hours of total student workload (CNPS)	90				
Form of crediting	crediting with grade				
For group of courses mark (X) final course					
Number of ECTS points	3				
including number of ECTS points for practical (P) classes					
including number of ECTS points for direct teacher-	80				

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[28] Principles of general and organic chemistry. [29] Principles of biochemistry.

SUBJECT OBJECTIVES	
C1	Acquainting of students with the basics of experimental research methodology.
C2	Acquainting with selected aspects of research and experimental analysis and interpretation of results, errors and measurement uncertainty, creating of models and hypotheses.
C3	Acquainting with selected experimental methods used in chemistry and biochemistry.
C4	Learning of conducting of laboratory notes and writing of research reports.
C5	Learning of research organization and planning of the experiment.
C6	Acquainting with databases and programs for data analysis.
C7	Acquainting with problems of ethics in science.

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

Person who pass the course:

PEK_W01 – knows the basic types of scientific methods.

PEK_W02 – knows the basic databases

PEK_W03 – knows how to properly conduct experimental notes and write a research report

PEK_W04 – knows the basic research methods used in chemistry and biochemistry

PEK_W05 – knows the basic aspects of ethics in science and research PEK_W06 – is able to formulate the research problem. PEK_W07 – is able to plan the experiment and analyze the obtained results

PROGRAMME CONTENT		
Form of classes - lecture		Number of hours
Lec 1	Basic concepts and types of scientific methods.	2
Lec 2	Choosing your research area. Pointing the research subjects/problems.	2
Lec 3	Research methods in chemistry.	2
Lec 4	Research methods in biochemistry.	2
Lec 5	Creating the scientific laws and models construction.	2
Lec 6	Results/data interpretation and analysis.	2
Lec 7	Measurement errors and their types. Uncertainty of measurement.	2
Lec 8	Writing the experimental report and making useful experimental notes.	2
Lec 9	Testing the hypotheses.	2
Lec 10	Validation of research method.	2
Lec 11	Planning a safe experiment.	2
Lec 12	Time and project management.	2
Lec 13	Databases and basic computer software for data analysis.	2
Lec 14	Organizing a successful research group.	2
Lec 15	Ethics in science and research.	2
	Total hours	**30**

TEACHING TOOLS USED	
N1	Lecture with multimedia presentation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F	PEK_W01- PEK_W07	Two essay
P= arithmetical mean of the grades		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[3] R. B. Burns, Introduction to research methods, SAGE Publications Ltd, 2000.
[4] C. Fini, A. Floridi, V. N. Finelli, Laboratory Methodology in Biochemistry, CRC Press, 1989.

SECONDARY LITERATURE:

[5] Any biochemistry and chemistry textbooks.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT
Methodology of experimental research
AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY
Biotechnology

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**	K2Abt_W02	C1	Wy1	N1
PEK_W02	K2Abt_W02	C6	Wy13	N1
PEK_W03	K2Abt_W02	C4	Wy8	N1
PEK_W04	K2Abt_W02	C3	Wy3,Wy4	N1
PEK_W05	K2Abt_W02	C7	Wy15	N1
PEK_W06	K2Abt_W02	C5	Wy2	N1
PEK_W07	K2Abt_W02	C2,C5	Wy5-7, Wy9-12, Wy14	N1

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Faculty of Chemistry

SUBJECT CARD

Name in Polish **Nowoczesne tendencje zarządzania**

Name in English **Modern tendencies in management**

Main field of study (if applicable): …….

Specialization (if applicable): ……..

Level and form of studies: 2nd level, full-time

Kind of subject: university-wide

Subject code **ZMZ000383**

Group of courses NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15				
Number of hours of total student workload (CNPS)	30				
Form of crediting	crediting with grade				
For group of courses mark (X) final course					
Number of ECTS points	1				
including number of ECTS points for practical (P) classes					
including number of ECTS points for direct teacher-student contact (BK) classes	0,5				

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. None
2.
3.

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SUBJECT OBJECTIVES

C1: To provide students with knowledge of the nature, characteristics and directions of development of management and the challenges facing the modern management.

C2: To familiarize students with selected concepts and methods that are regarded as useful in the management of the modern enterprise. To present the evidence and barriers to the implementation of these methods, the basic principles, theirs components, and the advantages and disadvantages as well.

C3: To provide students with knowledge about the values important for modern enterprises that are taken into consideration in the management process.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

Student:

PEK_W01: has a basic knowledge of management processes: can explain the nature and object management and identify the basic problems of management.

PEK_W02: has knowledge of the characteristics and directions of the contemporary management development and of the values relevant to the modern enterprise taken into consideration in the management process.

PEK_W03: Knows the selected modern management concepts and methods (including TQM, CSR, outsourcing, controlling, benchmarking, CRM, lean management, BPR, process management, knowledge management, JIT, virtual organization and learning organization, change management, projects management, time based management, BSC). Recognizes and understands their nature, objectives, conditions and barriers to their implementation, their basic components, and the advantages and disadvantages of their implementation as well.

PROGRAMME CONTENT

Form of classes - lecture		**Number of hours**
Lec 1	Introduction: the nature, object and history of management.	2
Lec 2	Challenges for the contemporary management (globalization and changes in the business environment, the idea of sustainable development). Characteristics and trends of contemporary management (focusing on customers, process approach, network cooperation, etc.).	2
Lec 3 – Lec 5	Chosen modern management concepts and methods (CSR, outsourcing, controlling, benchmarking, CRM, lean management, BPR, process management, knowledge management, JIT, virtual organization and learning organization, TQM, value based management, BSC etc.)	6
Lec 6 – Lec 7	The values relevant to the modern enterprise taken into account in the management process (management of cultural diversity, management of small businesses, family business management, management of information systems, management of communication in organization, time management, business ethics etc.)	4
Lec 8		1
	Total hours	15

Form of classes - class		**Number of hours**
Cl 1		
Cl 2		
Cl 3		
	Total hours	

Form of classes - laboratory		**Number of hours**
Lab 1		
Lab 2		
Lab 3		

	Total hours	

Form of classes - project		Number of hours
Proj 1		
Proj 2		
Proj 3		
	Total hours	

Form of classes - seminar		Number of hours
Sem 1		
Sem 2		
Sem 3		
	Total hours	

TEACHING TOOLS USED

N1. Presentation of knowledge in the form of direct communication (lecture) - audio-visual media (slides, computer projector)
N2. Lecture materials (synthesis) available in electronic form.
N3. Case studies.

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1	PEK_W01 – PEK_W03	Written colloquium
C==**100% F1**		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[5] Brilman J.: Nowoczesne koncepcje i metody zarządzania, Polskie Wyd. Ekonomiczne, Warszawa 2002.
[6] *Współczesne metody zarządzania w teorii i praktyce*, pod red. M. Hopeja i Z. Krala, Oficyna Wydawnicza PWr, Wrocław 2011.
[7] Zimniewicz K., *Współczesne koncepcje i metody zarządzania*, PWE, Warszawa 2009.

SECONDARY LITERATURE:

[6] Bielski M.: *Podstawy teorii organizacji i zarządzania*, C. H. Beck, Warszawa 2004.
[7] Drucker P.F., *Praktyka zarządzania*, Wyd. Nowoczesność, Warszawa 1994.
[8] *Podstawy nauki o przedsiębiorstwie*, red. J. Lichtarski, Wydawnictwo Akademii Ekonomicznej we Wrocławiu, Wrocław 2007.
[9] *Zarządzanie. Teoria i praktyka*, pod red. A.K. Koźmińskiego i W. Piotrowskiego, PWN, Warszawa 1995.

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

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT
Modern tendencies in management
AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY ……..
AND SPECIALIZATION ……..

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
PEK_W01 (knowledge)				
PEK_W02				
PEK_W03				
…				
PEK_U01 (skills)				
PEK_U02				
…				
PEK_K01 (competences)				
PEK_K02				
…				

** - enter symbols for main-field-of-study/specialization educational effects
*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Dynamika Molekularna**
Name in English	**Molecular Dynamics**
Main field of study (if applicable)	**bionanotechnology**
Specialization (if applicable)	**bioinformatics**
Level and form of studies:	**~~1st~~/ 2nd* level, full-time / ~~part-time~~***
Kind of subject	**obligatory / ~~optional / university-wide~~***
Subject code	**CHC024052**
Group of courses	**~~YES~~ / NO***

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30		30		
Number of hours of total student workload (CNPS)	120		60		
Form of crediting	crediting with grade		crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	4		2		
including number of ECTS points for practical (P) classes			2		
including number of ECTS points for direct teacher-	1		1		

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[1] Basic knowledge of physical chemistry (1st level)
[2] Basic knowledge of calculus (1st level)

SUBJECT OBJECTIVES	
C1	Basic knowledge of statistical thermodynamics
C2	Design of force fields and basics of molecular dynamics (MD)
C3	Algorithms used in molecular dynamics
C4	Preparation and running of molecular dynamics simulations

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEK_W01 – Basic concepts and laws of statistical thermodynamics

PEK_W02 – Potential energy form for a force field and understanding the physical meaning of each term

PEK_W03 – Methods to search for a global minimum in biological systems

PEK_W04 – How to choose suitable algorithms for molecular dynamics simulations

PEK_W05 – Algorithms to control temperature and pressure

PEK_W06 – Algorithms to calculate free energy within molecular dynamics framework

PEK_W07 – Analysis of MD results

Relating to skills:

PEK_U01 – Practical knowledge of Linux operating sytem

PEK_U02 – Practical knowledge of specific software to visualize and manipulate

biomolecules PEK_U03 – Practical knowledge of preparing input files and run and analyze simple minimization and MD simulations PEK_U04 – Practical knowledge on how to prepare and run basic MD simulations for proteins

PROGRAMME CONTENT		
Form of classes - lecture		Number of hours
Lec 1	**Basic concepts.** Molecular mechanics vs. quantum mechanics. Limitations of molecular mechanics. How good can MD be? - comparison with experimental results. The choice of a time step in MD simulations to describe various phenomena.	2
Lec 2	**Introduction to statistical thermodynamics.** Permutations and configurations. Probability theory in chemistry. Stirling approximation. Maxwell distribution. Partition function. Significance of Boltzmann distribution in chemistry. Statistical ensembles. Canonical ensemble. Canonical partition function: translational, rotational, vibrational and electronic terms.	2
Lec 3	**Introduction to statistical thermodynamics – part 2.** Internal energy and partition function: translational, rotational, vibrational and electronic contributions. Heat capacity and partition function.Entropy and partition function. Boltzmann equation and canonical partition function. Residual entropy. Free energy and equilibrium constant and partition function.	2
Lec 4	**Quiz 1.** Statistical thermodynamics	2
Lec 5	**Force field – part 1.** Definition of force field. Potential energy in force field. Bonding and non-bonding terms of potential. Harmonic and Morse potential. Mixed terms. Point charge model. RESP procedure. Buckingham and Lennarda-Jones potentials. Combination rules to create van der Waals parameters. Scaling of non-bonding potentials. Evaluation of cpu time in calculations of various potential energy terms.	2

Lec 6	**Force field – part 2.** All-atom and united-atom force fields. Transferability of force field parameters among different force fields. Accuracy of various force fields.	2
Lec 7	**Preparation of input files for MD simulations.** GROMACS options. How to choose an initial structure? A choice of a force field. Phases of MD procedure: minimization, heating, equilibration and production phase.Preparation of all required input files for MD simulations.	2
Lec 8	**Methods of searching for global minimum in biomolecules.** Methods for energy minimization. Levinthal paradox. Local and global minima in biosystems. Monte-Carlo method. Simulated annealing method. Genetic algorithm. Chain growth method. Homology modelling. Distance-geometry algoritm. Fragment-based algorithm.	2
Lec 9	**MD algorithms – part 1.** Determinism. Lyapunov instability. Newton's formalism. Lagrange's formalism. Hamilton's formalism. Integer algorithms: Euler, Verlet, velocity-Verlet, leap-frog, predictor-corrector. What are the features of a good algorithm? What are the criteria of choosing an optimal algorithm?	2
Lec 10	**MD algorithms– part 2.**Time step. Shake and rattle algorithms. Multiple time-step method. Liouville operator.	2
Lec 11	**MD algorithms– part 3.** Periodic boundary conditions. Minimum image convention. Cut-off technique. Switching i shifting functions. Neighbor list, cell list and Verlet list methods.	2
Lec 12	**MD algorithms – part 4.** Temperature and pressure in MD. Methods to control temperature in MD: stochastic, weak-coupling, strong-coupling, Nose-Hoover. Methods to control pressure in MD: volume scaling, Berendsen, Nose-Hoover and Andersen.	2
Lec 13	**Free energy in MD.** Algorithms to calculate free energy in MD: thermodynamic perturbation, thermodynamic integration and linear interaction energy. Free energy of solvation. Free energy binding of inhibitor to enzyme.	2
Lec 14	**Analysis of MD results.** Average quantities – temperature and pressure. Fluctuations: isobaric and isochoric heat capacity. Structural quantities: pair distribution function and static structure factor. Dynamic quantities: diffusion coefficient, velocity autocorrelation function, dynamic structure factor, MSD. Dipole autocorrelation function.	2
Lec 15	**Quiz 2.** MD algorithms	2
	Total hours	**30**

Form of classes - laboratory		Number of hours
Lab 1	Requirements to pass a laboratory course.	2
Lab 2	Basic Linux commands.	2
Lab 3	Basic commands ot 'vim' text editor.	2
Lab 4	Z matrix preparation for simple molecules using Molden software.	2
Lab 5	Basic commands of VMD visualization software.	2
Lab 6	VMD as a tool to analyze results of MD simulations.	2
Lab 7	Preparation of input files to simulate 216 water molecules using GROMACS. Calculations and analysis of results.	2
Lab 8	Preparation of input files to simulate 216 methanol molecules using GROMACS. Calculations and analysis of results.	2
Lab 9	Preparation of input files to simulate a mixture of water and methanol molecules using GROMACS. Calculations and analysis of results.	2
Lab 10	Preparation of input files to simulate a ribonuclease S-peptide using MD.	2
Lab 11	Analysis of MD results for ribonuclease S-peptide in water.	2
Lab 12	Preparation of input files for minimization procedure of BPTI protein in water.	2
Lab 13	MD simulations of BPTI protein in water – heating, equilibration and production phases of MD.	2
Lab 14	Trajectory analysis of MD simulations of BPTI protein in water: RMSD, RMSF, kinetic energy, temperature, pressure, Ramachandran plot, hydrogen bonds and salt bridges, density of protein and water.	2
Lab 15	How does the change in time step, force field, deviation in Cartesian coordinates, the choice of an algorithm and van der Waals cut-off affect the physical properties of S-peptide? Analysis of the results.	2
	Total hours	**30**

TEACHING TOOLS USED	
N1	Lecture with multimedia presentation
N2	Solving pratice problem sets
N3	Usage of software
N4	Preparation of reports

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1	PEK_W01	Quiz 1
F2	PEK_W02 – PEK_W07	Quiz 2
P (laboratory)	PEK_U01 – PEK_U05	Report
P (lecture) = 3.0 if (F1 + F2) = 50-60% max. no of poins **3.5 if (F1 + F2) = 61-70% max. no of poins** **4.0 if (F1 + F2) = 71-80% max. no of poins** **4.5 if (F1 + F2) = 81-90% max. no of poins** **5.0 if (F1 + F2) = 91-99% max. no of poins** **5.5 if (F1 + F2) = 100% max. no of poins.**		

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE: [1]. D. Frenkel, B. Smith "Understanding Molecular Simulation", Academic Press, 2001. [2] J.M. Haile "Molecular Dynamics Simulation: Elementary Methods", Wiley-Interscience, 1997. **SECONDARY LITERATURE:** [1] M. P. Allen, D. J. Tildesley "Computer Simulation of Liquids", Oxford University Press, 1989.

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Molecular dynamics

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology, specializatoin: Bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**	S2bt5_W02	C1	Wy1-Wy4	N1, N2
PEK_W02	S2bt5_W02	C2	Wy5-Wy6	N1
PEK_W03	S2bt5_W02	C2	Wy7-Wy8	N1
PEK_W04	S2bt5_W02	C3	Wy9–Wy11	N1
PEK_W05	S2bt5_W02	C3	Wy12	N1

PEK_W06	S2bt5_W02	C3	Wy13	N1
PEK_W07	S2bt5_W02	C3	Wy14– Wy15	N1
(skills) **PEK_U01**	S2bt5_U02	C4	La1 – La3	N3
PEK_U02	S2bt5_U02	C4	La4 – La6	N3
PEK_U03	S2bt5_U02	C4	La7-La9	N3,N4
PEK_U04	S2bt5_U02	C4	La10– La15	N3, N4

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Modelowanie molekularne**
Name in English	**Molecular modeling**
Main field of study (if applicable)	**Biotechnology**
Specialization (if applicable)	**Bioinformatics, Medicinal Chemistry**
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**CHC024006**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15		30		15
Number of hours of total student workload (CNPS)	30		60		15
Form of crediting	crediting with grade		crediting with grade		crediting with grade
For group of courses mark (X) final course					
Number of ECTS points	2		2		1
including number of ECTS points for practical (P) classes			1		
including number of ECTS points for direct teacher-	2		1		1

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[30] Basic knowledge of atomic and molecular structure concepts
[31] Basic knowledge of analytic geometry
[32] Basic knowledge of computer science
[33] Basic knowledge of organic chemistry

SUBJECT OBJECTIVES	
C1	Teaching construction of 3-D molecular models
C2	Teaching elementary quantum chemistry methods
C3	Teaching elementary concepts of the theory of intermolecular interactions
C4	Teaching modeling techniques of molecular aggregates
C5	Teaching modeling chemical reactions

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEK_W01 – knowledge of construction of 3-dimensional molecular models and their transformations

PEK_W02 - knowledge of elementary molecular modeling methods and limits of their applications.

PEK_W03 - knowledge of major components of intermolecular interaction energy

PEK_W04 - knowledge of modeling drugs and biocatalysts

Relating to skills:

PEK_U01 – ability of construction of 3-D molecular model starting from assumed

hybridization type PEK_U02 – ability to predict molecular structure and properties PEK_U03 - ability to predict possibile structures of molecular aggregates PEK_U04 - ability to analyse protein-ligand interactions PEK_U05 - ability to model dynamic properties of molecular aggregates

PROGRAMME CONTENT		
Form of classes – lecture		Number of hours
Wy1	Basic concepts. Interdisciplinary charakter of molecular modeling. Typical molecular modeling tasks. Molecular structure sources. Algorithms used in construction of 3-D molecular models with examples. Hybridization. Coordinate transformations. Basic concepts of molecular graphics. Visualization techniques. Literature review.	2
Wy2	Basic concepts of quantum chemistry. Review of quantum chemistry computational methods. Hueckel Molecular Orbitals and ab intio methods. Theoretical prediction of physical properties and structure.	2
Wy3	Construction of molecular models – exercise and test	2
Wy4	Basic concepts of the theory of intermolecular interactions. Perturbation theory. Characteristics of major components of intermolecular interaction components.	2
Wy5	Hydrogen bonding. Molecular charge distribution and electrostatic models. Force fields.	2
Wy6	Predicting properties and structure of molecular aggregates – exercises and test.	2
Wy7	Modeling interactions In receptors and enzyme active centers. Drug design techniques. Molecular dynamice. Homology modeling.	2
Wy8	Analysis of enzyme catalytic activity and biocatalyst design.	1
	Total hours	15

Form of classes - laboratory		Number of hours
La1	Introduction and lab organization.	2
La2	Molecular structure graphical representations	2
La3	Preparing molecular dynamice simulations	2
La4	Analysis of molecular dynamice trajectories	2
La5	Computational task #1.	2
La6	Z matrix representation of molecular structure - introduction to Molden program.	2
La7	Theoretical introduction to quantum chemical calculations of molecular structure.	2
La8	Geometry optimization calculation of molecular properties.	2
La9	Analysis and visualization of results of quantum chemical calculations. Analysis of normal vibrations.	2
La10	Noncovalent interactions. Structure of aggregates and interaction energy calculations.	2
La11	Computational task #2.	2
La12	Computational task #3.	2
La13	Introduction to theoretical methods used in silico docking.	2
La14	Receptor-ligand docking simulations	2
La15	Computational task #4	2
	Total hours	**30**

Form of classes - seminar		Number of hours
Se1	Student seminars: protein structure prediction, homology modeling	2

Se2	Student seminars: superimposing molecules, docking, predicting protonation state	2
Se3	Student seminars: modeling receptors, sensors, molecular switches, molecular motors	2
Se4	Student seminars: use of genetic algorithms and neural nets in molecular modeling	2
Se5	Student seminars: drug design techniques	2
Se6	Student seminars: modeling IR, Raman, UV, NMR spectra	2
Se7	Student seminars: modeling chemical Reaction and transition states	2
Se8	Student seminars: biokatalyst design	1
	Total hours	15

TEACHING TOOLS USED	
N1	Lecture with multimedia presentation
N2	Solving problems
N3	Use of software
N4	Student multimedia presentation
N5	Preparing report

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1 (lecture)	PEK_U01	Test #1
F2 (lecture)	PEK_U02 PEK_U03	Test #2

C (lecture) = F1 + F2		
C (seminar)	PEK_W01 PEK_W02 PEK_W03 PEK_W04	Student multimedia presentation
F3 (lab)	PEK_U05	Partial report #1
F4 (lab)	PEK_U01 PEK_U02	Partial report #2
F5 (lab)	PEK_U02 PEK_U03	Partial report #3
F6 (lab)	PEK_U04	Partial report #4
C (lab) = F3 + F4 + F5 + F6		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[8] L. Piela, Quantum Chemistry Ideas, Elsevier, 2010

[9] A.R. Leach, Molecular Modeling:Principles and Applications, 2 wydanie, Prentice Hall, 2001

[10] H.D. Hotje, Molecular modeling. Basic principles and applications, 3 wydanie, Wiley, 2008

[11] T. Schlick, Molecular modeling and simulation, Springer, 2002.

SECONDARY LITERATURE:

[10] F. Jensen, Introduction to computational chemistry, Wiley, 2006 (2-nd Ed)

[11] J.M. Goodman, Chemical Applications of Molecular Modeling, RSC, 1999.

[12] J.P. Doucet, J. Weber, Computer-Aided Molecular Design, 1996,Academic Press, 1996

[13] G.H. Grant, W.G. Richards, Computational chemistry, Oxford Sci. Publ., 1995

SUBJECT SUPERVISOR

(NAME AND SURNAME, E-MAIL ADDRESS)

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Molecular modeling

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**	T2A_W02 T2A_W03 **X2A_W02 X2A_W03**	C1	Wy1,Wy3 Se1, Se2	N1,N2, N4
PEK_W02	T2A_W02 T2A_W03 **X2A_W02 X2A_W03**	C2	Wy2,Wy6 Se3, Se4	N1,N2, N4
PEK_W03	T2A_W02 T2A_W03 **X2A_W02 X2A_W03**	C3	Wy4, Wy6 Se5, Se6	N1,N2, N4
PEK_W04	T2A_W02 T2A_W03 **X2A_W02 X2A_W03**	C4, C5	Wy7, Wy8 Se7,Se8	N1,N4
(skills) **PEK_U01**	T2A_U01 T2A_U08 T2A_U11 InzA_U01	C1	La2, La6	N2, N3, N5
PEK_U02	T2A_U01 T2A_U08 T2A_U11 **X2A_U03 X2A_U04** InzA_U01	C2	La7, La8, La9, La11	N2, N3, N5
PEK_U03	T2A_U01 T2A_U08 T2A_U11 **X2A_U03 X2A_U04** InzA_U01	C3	La10, La12	N3, N5
PEK_U04	T2A_U01 T2A_U08 T2A_U11 **X2A_U03 X2A_U04** InzA_U01	C4	La13, La14, La15	N3, N5
PEK_U05	T2A_U01 T2A_U08 T2A_U11 **X2A_U03 X2A_U04** InzA_U01	C4	La3, La4, La5	N3, N5

Wrocław University of Technology
FACULTY Chemistry

SUBJECT CARD

Name in Polish **Sieci i stacje robocze z systemem unix**
Name in English **Networks and workstations with unix system**
Main field of study (if applicable): …biotechnology
Specialization (if applicable): …bioinformatics..
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code INC024002l
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		

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. English - basic level
2. Basic computer skills

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SUBJECT OBJECTIVES

C1 Learning the mechanisms that govern unix systems
C2 Developing skills for using unix systems at unassisted administration level
C3 Understanding the rules for network based on the internet protocol
C4 Learning how to use network services in unix system and how to make them available for use.

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEK_W01 knows the mechanisms for running and configuring a unix system

PEK_W02 knows the relationship between user's account and user's and group's identifiers; understands their connection with rights to perform various operations in the system

PEK_W03 knows the basic rules of network based on the internet protocol (IP version 4) and the connection between the name and internet address

PEK_W04 knows the mechanisms of using and making available network services, which make use of TCP and UDP transport protocols.

relating to skills:

PEK_U01 can run programs from the command line, in text terminal

PEK_U02 can create files of various types, perform basic operations on files, use a text editor, handle compressed files and tar archives

PEK_U03 can write an inittab file and simple scripts responsible for starting the system, chek the consistency of a filesystem and attach it to the directory tree

PEK_U04 can add and remove user accounts, change passwords and assign users to groups; can write session scripts (bash shell)

PEK_U05 can assign the network address to network interface, build the routing table, create local list of address-name relationships and prepare the system for using the DNS service

PEK_U06 can use, in unix system, the services of remote terminal (telnet, ssh), copying files (ftp, sftp, scp), electronic mail and ftp; can make these services available and constrict the access to them, via entries in hosts.allow and hosts.deny files

PEK_U07 can run local and remote graphical applications in the X window system

PEK_U08 can use documentation for programs, available in unix system

PROGRAMME CONTENT	
Form of classes - laboratory	
Lab 1	Programs and processes. Parent and child processes, system mechanisms for running programs and process termination. Signals. User's and group's identifiers - introduction of mechanisms regulating access rights to various system resources.
Lab 2	Files and file types: normal, directories, special (character and block devices), files representing communication channels (sockets and named pipes). Normal pipes and their similarity to files. The notion of a filesystem, hard and symbolic links. Review of programs for various file operations, including short introduction to the vi editor.
Lab 3	Running the linux kernel under control of the QEMU emulator. Creation of a file representing hard disk, partitioning and creation of filesystem. Archives created with the tar program. Installation of minimal set of programs, needed for bootstrapping the system.
Lab 4	Duties of the program running with process identifier equal to 1. Configuration of the init program (implementation: sysvinit) - the inittab file. Review of tasks performed at the system's initialization stage.

Lab 5	Checking of filesystems' consistency and attaching filesystems to the directory tree. Mount and umount programs, the /etc/fstab file. Shared libraries.
Lab 6	User accounts - entries in the /etc/passwd file, relationship of names with user identifiers, home directories, encryption and storing of passwords. System and personal session scripts. Creation of groups (the /etc/group file). Programs: su and newgrp.
Lab 7	IP address, address' class, structure of an address within given network segment (network mask). Assignement of IP address to the network interface, with the ifconfig program. The loopback interface. Creation of the routing table with the route program.
Lab 8	Internet names, name-address relationship. Methods for translating names to addresses and addresses to names: local list in the /etc/hosts file and the DNS network service.
Lab 9	TCP and UDP transport protocols. The notion of network socket. Assignement of network services to port numbers (/etc/services file). Rules of making services available by the inetd program.
Lab 10	Constricting remote access to network services - mechanisms and configuration of the TCP wrappers software (tcpd program and library code) by access control lists in /etc/hosts.allow and /etc/hosts.deny files.
Lab 11	Working in a remote system - services of remote terminal (telnet and ssh) and file transfer (ftp, scp, sftp). Reasons for using encrypted communication channels.
Lab 12	Electronic mail - MTA and MUA programs, running an MTA program (smail) and using the mutt mail client (MUA). Basic rules for securing the mail server (MTA).
Lab 13	The WWW server - basic configuration of the boa program, creation of simplest WWW pages in the HTML language. Text WWW browser - lynx.
Lab 14	The X window system - graphical environment with client-server architecture.
Lab 15	Crediting
	Total hours: 30

TEACHING TOOLS USED
N1. Demonstration N2. Practical exercises, under teacher's control N3. Practical exercises , with a simple problem to be solved single-handedly by the student

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1	PEK_U01-U08	practical exercises (up to 25 points)

F2	PEK_W01-W04, PEK_U02-U06	written test (up to 75 points)
F3	PEK_W01-W04, PEK_U02-U06	outstanding knowledge or skills (up to 10 points)

P=F1+F2+F3; concluding grade
50 <= P < 60 3.0
60 <= P < 70 3.5
70 <= P < 80 4.0
80 <= P < 90 4.5
90 <= P < 100 5.0
P >= 100 5.5

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] ªleen Frisch, UNIX: administracja systemu, O'Reilly & Associates, wydawnictwo RM, Warszawa 1997

SECONDARY LITERATURE:

[1] Craig Hunt, **TCP/IP** : administracja sieci. wydawnictwo RM, Warszawa 2003

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Networks and workstations with unix system

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

biotechnology

AND SPECIALIZATION bioinformatics

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
PEK_W01 (knowledge)		C1	Lab1-Lab14	N1,N2,N3
PEK_W02		C1,C2	Lab1, Lab2, Lab6	N1,N2
PEK_W03		C3	Lab7, Lab8	N1,N2
PEK_W04		C1,C4	Lab9-Lab13	N1,N2,N3
PEK_U01 (skills)	S2Abt5_U03	C1	Lab1	N1,N2
PEK_U02	S2Abt5_U03	C1,C2	Lab2,Lab3	N1,N2
PEK_U03	S2Abt5_U03	C1,C2	Lab4,Lab5	N1,N2,N3
PEK_U04	S2Abt5_U03	C1,C2	Lab6	N1,N2
PEK_U05	S2Abt5_U03	C3	Lab7,Lab8	N1,N2
PEK_U06	S2Abt5_U03	C3,C4	Lab9-Lab13	N1,N2,N3
PEK_U07	S2Abt5_U03	C1,C2,C3,C4	Lab14	N1,N2
PEK_U08	K2Abt_U05	C1,C2	Lab1,Lab2	N1,N2

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

FACULTY OF CHEMISTRY / DEPARTMENT of HUMANITIES

SUBJECT CARD

Name in Polish **Filozofia nauki i techniki**

Name in English **Philosophy of science and technology**

Main field of study (if applicable):

Specialization (if applicable):

Level and form of studies: 2nd level, full-time

Kind of subject: obligatory

Subject code FLC024004

Group of courses NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15				
Number of hours of total student workload (CNPS)	30				
Form of crediting	crediting with grade				
For group of courses mark (X) final course					
Number of ECTS points	1				
including number of ECTS points for practical (P) classes					
including number of ECTS points for direct teacher-student contact (BK) classes	0.5				

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Non

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SUBJECT OBJECTIVES

C1 To acquaint students with specificity of philosophical reflection about science and technology.
C2 Systematize and deepen the knowledge of the basic methods of inference that regulate and organize our knowledge.
C3 Performance considerations of engineer's activity and to present the issue of social responsibility in science and technology.

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEK_ HUM W07 The student gains knowledge of the basic methods of inference (deduction, induction and abduction).

PEK_ HUM W08 The student has knowledge that is essential to understanding and interpreting social and philosophical considerations of engineer's activity.

Relating to social competences:

PEK_HUM K01 The student is aware of the importance of understanding non-technical aspects and of engineer's activity, its consequences and responsibility for undertaken decisions.

PROGRAMME CONTENT		
Form of classes - lecture		**Number of hours**
Lec 1,2	What is the science and technology? The basic concepts and principles of the philosophy of science and philosophy of technology.	2
Lec 3	The main criteria of scientific knowledge.	1
Lec 4	The tradition of doing science from the point of view of the theory	1
Lec 5	The tradition of doing science from the point of view of the experiment.	1
Lec 6	The basic methods of inference – induction.	1
Lec 7	The basic methods of inference – deduction.	1
Lec 8	The basic methods of inference – abduction.	1
Lec 9,10	The main objectives and functions of science and technology from the point of view of classical philosophy of science.	2
Lec 11	The main aims and functions of science and technology from the point of view of the sociology of scientific knowledge.	1
Lec 12, 13	The concept of science laboratory.	2
Lec 14, 15	The problem of social responsibility of science and technology.	2
	Total hours	15

Form of classes – class		**Number of hours**
Cl 1		
Cl 2		
Cl 3		
Cl 4		
..		
	Total hours	

Form of classes – laboratory		**Number of hours**
Lab1		
Lab2		
Lab3		
Lab4		
Lab5		
…		
	Total hours	

Form of classes – Project	**Number of h**

		o u r s
Proj1		
Proj2		
Proj3		
Proj4		
…		
	Total hours	

Form of classes – seminar		**Number of hours**
Sem1		
Sem2		
Sem3		
…		
	Total hours	

TEACHING TOOLS USED

N1. Multimedia presentation.
N2. Lecture
N3. Interactive lecture

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation(F – forming (during semester), P – concluding (at semester end)	Educationaleffectnumber	Way of evaluating educational effect achievement
F1	PEK_ HUM W07 PEK_ HUM W08 PEK_ HUM K01	Passing test, active participation in lectures
P=F1		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[12] E. Agazzi, *Dobro, zło i nauka. Etyczny wymiar działalności naukowo-technicznej*, Warszawa 1997;
[13] S. Blackburn, *Oksfordzki słownik filozoficzny*, Warszawa 2004;
[14] A. Chalmers, *Czym jest to, co zwiemy nauką*, Wrocław 1997;
[15] R. M. Chisholm, *Teoria poznania*,1994;
[16] Ch. Frankfort- Nachmiast, D. Nachmiast, *Metody badawcze w naukach społecznych*, Poznań 2001;
[17] A. Grobler, *Metodologia nauk*, Kraków 2004;
[18] M. Heidegger, *Budować, mieszkać, myśleć*, Warszawa 1977;
[19] T. Kuhn, *Dwa bieguny*, Warszawa 1985;
[20] B. Latour, *Polityka natury*, Warszawa 2009;
[21] K.R. Popper, *Wiedza obiektywna*, Warszawa 1992;

[22] J. Woleński, *Epistemologia*, Warszawa 2005.

SECONDARY LITERATURE:

[14] [1] D. Sobczyńska, P. Zeidler*, Nowy eksperymentalizm. Teoretycyzm. Reprezentacja,* Poznań 1994,
[15] P. Zeidler*, Spór o status poznawczy teorii*, Poznań 1992.

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT **Philosophy of science and technology** AND EDUCATIONAL EFFECTS IN THE FIELD OF TECHNICAL SCIENCES

Subject educational effect	**Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)****	**Subject objectives*****	**Programme content*****	**Teaching tool number*****
PEK_ HUM W07; **PEK_ HUM W08 (knowledge)**	**T2A_W07** **T2A_W08**	C1, C2	Lec1-Lec9	N1, N2
PEK_HUMK01 (competences)	**T2A_K01**	C1	Lec1, Lec10-Lec15	N1, N2, N3

** - enter symbols for main-field-of-study/specialization educational effects
*** - from tableabove

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish **Systemy Zarządzania Jakością**

Name in English **Quality Management Systems**

Main field of study (if applicable): *Biotechnology*

Specialization (if applicable): *Bioinformatics*

Level and form of studies: ~~1st~~/ 2nd* level, full-time / ~~part-time~~*

Kind of subject: obligatory / ~~optional~~ / ~~university-wide~~*

Subject code ZMC024003w

Group of courses ~~YES~~ / NO*

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15				
Number of hours of total student workload (CNPS)	30				
Form of crediting	Examination / ~~crediting with grade~~*	Examination / crediting with grade*	Examination / crediting with grade*	Examination / crediting with grade*	Examination / crediting with grade*
For group of courses mark (X) final course					
Number of ECTS points	1				
including number of ECTS points for practical (P) classes	0				
including number of ECTS points for direct teacher-student contact (BK) classes	1				

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Intruductory statistical data analysis

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SUBJECT OBJECTIVES

C1 Understanding of basic rules of work organization and integrated management system in technical fields and other activities.

C2 General knowledge of statistical process control. Working knowledge of the concepts of uncertainty of measurements.

C3 Understanding of basic concepts of chemical metrology.

SUBJECT EDUCATIONAL EFFECTS
relating to knowledge: PEK_W01 Knowledge of the origins and basics concepts of quality management PEK_W02 Knowledge of statistical methods for data analysis and hypothesis testing PEK_W03 Knowledge of the requirements for the validation of test methods PEK_W04 Knowledge of requirements for ensuring traceability of measurements relating to skills: PEK_U01 Design and documentation of the quality management system elements PEK_U02 Ability to apply the tools of description, analysis and planning of processes PEK_U02 Ability to apply basic tools of statistical process control

PROGRAMME CONTENT		
Form of classes - lecture		**Number of hours**
Lec 1	Quality management systems – introduction and historical outline	2
Lec 2	Conformity assessment systems	2
Lec 3	Management system in testing laboratory: Organization and management system. Control of nonconforming work or departures from the policies and procedures in the management system.	2
Lec 4	Management system in testing laboratory: Test and calibration methods and method validation.	3
Lec 5	Management system in testing laboratory: Estimation of uncertainty of measurement. Statistical hypothesis testing.	3
Lec 6	Management system in testing laboratory: Measuring equipment and measurement traceability.	1.5
Lec 7	Management system in testing laboratory: Assuring the quality of test results and reporting the results.	1.5
	Total hours	15

TEACHING TOOLS USED
N1. Lecture in the form of presentation N2. Learning management system Moodle

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement

C The exam in the form of a written test

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE:
[34] D. Hoyle *„Quality Management Essentials”,* Elsevier 2007;
[35] *„Complying with ISO 17025 - A practical guidebook”*, UNIDO, Vienna 2007;
[36] International standards EN ISO 9000 *„Quality management system – Fundamentals and vocabulary”* and EN ISO 9001 *„Quality management systems – Requirements”;*
[37] International standard EN ISO/IEC 17025 *“General requirements for the competence of testing and calibration laboratories.”*;
SECONDARY LITERATURE:
[38] EA-2/05 *„The Scope of Accreditation and Consideration of Methods and Criteria for the Assessment of the Scope in Testing”* (identical to ILAC-G18:2002);
[39] ILAC-G17:2002 *„Introducing the Concept of Uncertainty of Measurement in Testing in Association with the Application of the Standard ISO/IEC 17025”*;
[40] ILAC-G8:1996 *„Guidelines on Assessment and Reporting of Compliance with Specification”*;
[41] EURACHEM / CITAC Guide *„Traceability in Chemical Measurement”* (2003);
[42] *EURACHEM / CITAC Guide „Quantifying Uncertainty in Analytical Measurement”, 2nd Edition (2000)*
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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

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AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

……..

AND SPECIALIZATION ……..

Subject educational effect	**Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)****	**Subject objectives*****	**Programme content*****	**Teaching tool number*****
PEK_W01 (knowledge)				
PEK_W02				
…				
…				
PEK_U01 (skills)				
PEK_U02				
…				
PEK_K01 (competences)				
PEK_K02				
…				

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Racjonalne projektowanie leków**
Name in English	**Rational drug design**
Main field of study (if applicable)	**Biotechnology, Chemistry**
Specialization (if applicable)	**Bioinformatics, Medicinal Chemistry**
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**BTC024014**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30				
Number of hours of total student workload (CNPS)	90				
Form of crediting	drug design				
For group of courses mark (X) final course					
Number of ECTS points	3				
including number of ECTS points for practical (P) classes					

including number of ECTS points for direct teacher-student contact (BK) classes	1				

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

[43] Knowledge of basic organic chemistry

[44] Knowledge of basic biology

SUBJECT OBJECTIVES	
C1	Acquaintance with principles of design of biologically active substances
C2	To acknowledge economic aspects of drug design
C3	To ackonwlege principles of targetes therapy
C4	Acquaintance with principles of gene therapy

SUBJECT EDUCATIONAL EFFECTS

Student who finished the course:

Relating to knowkedge:

PEK_W01 – knows basic principles of dug design,

PEK_W02 – is able to propose suitable method of drug design in dependence of the level of knowledge about physiologic process involved,

PEK_W03 – understands economical aspects and time-limitations of design of drug design,

PEK_W04 – understands economic and physiologic outcomes of drug design.

Relating to skills:

PEK_U01 – is able to propose the method for the design of drug against certain illness.

PROGRAMME CONTENT		
Form of classes - lecture		Number of hours
Lec 1	**Economics of drug design and development.** Cost and time required to introduce new drug to the market. Generic drugs. Globalization.	2
Lec 2	**Randomized screening**. Historical perspective. Illustration of the opinion of Louyis Pasteur „*Fortune favors prepared minds*". Case studies.	2
Lec 3	**Natural products as a source of drugs.** History of the discovery of aspirin, morphine, artemisinin, quinine, penicillin and taxol. Current trends in natural drug research.**N**	2
Lec 4	**Choice of the target.** HIV as an example for choice of the target for drug design.	2
Lec 5	**Theory of structural analogy.** Historical perspective (sulfonamides). Direct similarity versus topological one with analogs of morphine and anti-influenza drugs as examples.	2
Lec 6	**Theory of structural analogy.** Chemical outlook, trics and "magic methods". Peptidomimetics.	2
Lec 7	**Three-dimensional structure of receptors as a basis for drug design. Construction of p**harmacophore. Computer-aided methods for drug design – QSAR and molecular modeling. Receptor flexability.	2
Lec 8	**Topological conformity.** Antagonists and agonists. Natural peptides as scaffolds.	2
Lec 9	**Covalent drugs – enzyme killers.** Overview of functional groups able for irreversivble bonding with proteins. Techniques of design of covalent drugs. Case studies.	2
Lec 10	**Suicidal drugs (suicide substrates) – Troian horses of enzymatic reactions.** Overview of the techniques leading to suicide substrates. Types od inhibition after conversion of suicidal drug into real inhibitor.	2
Lec 11	**Transition-state analogues.** Techniques used for the identification of transition state. Pauling's theory of the course of enzymatic reaction. Construction of transition-state analogues. Computer-aided techniques.	2
Lec12	**Selective complexation of metalloenzymes.** History of the discovery of captopril. Convertase as a target for anti-hypertensive drugs. Choice of ligand.	2

Lec13	**Drug targeting and delivery.** Invasive drug delivery (catheters, stents, microdialysers etc.). Nano-carriers – liposomes, vesicles, dendrimers, antibodies, proteins, nanopolymers and nanoparticels. Bacterial ghosts and virosomes. Prodrugs. Engineered metabolic activation. Targeted enzyme prodrug therapy.	2
Lec14	**Gene therapy.** Lacking gene delivery. Anti-sense oligonucleotides, siRNAs, rybosymes.	2
Lec15	Evaluation and grading of projects.	2
	Total hours	**30**

TEACHING TOOLS USED	
N1	Lecture and multimedia presentatio
N2	Preparation of project
N3	Interaktive system of consultation of project dvelopment

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
P (lecture)	PEK_W01 up to PEK_W04 PEK_U01	Drug design for chosen illness

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE: 14. K. M. Merz, Drug Design, structure and Ligand-Based Approaches, Cambridge University Press, 2010 15. Medicinal Chemistry and Drug Design, e d. D. Dnkici, Intech (open access), 2012 **SECONDARY LITERATURE:** 9. Design of Drugs: Basic Principles and applications, ed. J. H. Poupaert, Marcel Dekker, 2002 10. The Organic Chemistry of Drug Design and Drug Action, Academic Press, 2004 11. Virtual Screening. ed. M. O. Taha, Intech (open access), 2012 12. Drug Development – A Case study Based Insight intor Modern Startegies, Intech (open access), 2011

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Rational drug design

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology & Chemistry

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***

(wiedza) **PEK_W01** **PEK_W04**	S2Ach4_W01, S2Ach4_W10, S2bt5_W04	C1, C2	Lec1 – Lec 3	N-jeden
PEK_W01	S2Ach4_W02, S2Ach4_W10, S2bt5_W04	C1	Lec 2, Lec 3	N1
PEK_W03	S2Ach4_W10, S2bt5_W04, S2bt5_W02	C1,C3	Lec 2, Lec 5-Lec 14	N-jeden
PEK_U01	S2Ach4_W10, S2bt5_W04	C1	Lek15	N2, N3

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Informacja naukowa i techniczna w biotechnologii**
Name in English	**Retrieval of scientific and technical information**
Main field of study (if applicable)	**Biotechnology, Chemistry**
Specialization (if applicable)	**Bioinformatics, Medicinal chemistry**
Level and form of studies:	**2nd level, full-time**
Kind of subject	**obligatory**
Subject code	**INC024008**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)			15		
Number of hours of total student workload (CNPS)			30		
Form of crediting			crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points			1		
including number of ECTS points for practical (P) classes			1		

including number of ECTS points for direct teacher-student contact (BK) classes			0.5		

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[1] Basic computer science skills [2] Communication in English language

SUBJECT OBJECTIVES	
C1	Teaching practical use of computer network services
C2	Teaching basic concepts of scientific literature
C3	Teaching practical use of scientific literature databases
C4	Taching practical use of factographic databases
C5	Teaching basic concepts of funding scientific research
C6	Teaching basic concepts of ethical problems in science and engineering

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEK_W01 – knowledge of elementary computer network services

PEK_W02 - knowledge of the structure and preparing scientific publications and major scientific literature databases.

PEK_W03 - knowledge of the major factographic chemical and biotechnological databases.

PEK_W04 - knowledge of the major agencies funding research and development

PEK_W05 - knowledge of the typcal ethical problems in science and technology.

Relating to skills:

PEK_U01 – ability to transfer information between different computer systems
PEK_U02 – ability to construct complex search queries in scientific literature databases
PEK_U03 - ability to construct complex search queries in factographic databases
PEK_U04 - ability to find and analyse fellowship, job and practical training offers
PEK_U05 - ability to find currently funded reasearch grants on specific topics
PEK_U06 - ability to use plagiarism checkers

PROGRAMME CONTENT		
Form of classes – laboratory		Number of hours
La1	Initial information, assigning accounts, Structure and composing scientific texts	2
La2	Web of Science literature database, composing search queries	2
La3	Science citation index and various uses of impact factors	2
La4	Cambridge Structural Database, Analysis of structural information	2
La5	Research grant databases, fellowships, job and practical training offers, preparing CV and job interviews	2
La6	Patent databases	2
La7	Beilstein database and Reaxys, Chemical Abstracts database and Scifinder	2
La8	Ethical problems in science and industry, Individual report grading	1
	Total	15

TEACHING TOOLS USED	
N1	Multimedia presentation
N2	Solving problems

N3	Use of compter software to solve problems

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
C	PEK_U02	Final report maximum 100 score points grade 3.0 for 50-60 score points grade 3.5 for 61-70 score points grade 4.0 for 71-80 score points grade 4.5 for 81-90 score points grade 5.0 for 91-95 score points grade 5.5 for 96-100 score points
C	PEK_U03	
C	PEK_U04	
C	PEK_U05	

PRIMARY AND SECONDARY LITERATURE
PRIMARY LITERATURE: [1] D. Ridley, Finding scientific information – information retrieval, Wiley, 2002

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Retrieval of scientific and technical information in biotechnology

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Bioinformatics, medicinal chemistry

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme kontent***	Teaching tool number***
(knowledge) **PEK_W01**	T2A_U01 T2A_U07, X2A_U03	C1	La1	N1
PEK_W02	T2A_U01 T2A_U07, X2A_U03	C2	La2, La3	N2,N3
PEK_W03	T2A_U11 InzA_U05, X2A_U03	C3	La4, La6,La7	N1,N2,N3
PEK_W04	T2A_U11 InzA_U05, X2A_U03	C4	La5	N1,N3

PEK_W05	T2A_U11 InzA_U05, X2A_U03	C5	La8	N1,N3
(comptence) **PEK_U01**	T2A_U01 T2A_U07, X2A_U03	C1	La2	N2,N3
PEK_U02	T2A_U01 T2A_U07, X2A_U03	C3	La4,La6	N2,N3
PEK_U03	T2A_U01 T2A_U07, X2A_U03	C4	La5	N2,N3
PEK_U04	T2A_U01 T2A_U07, X2A_U03	C5	La5	N3
PEK_U05	T2A_U01 T2A_U07, X2A_U03	C5	La8	N1,N3

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above

Wrocław University of Technology **FACULTY OF CHEMISTRY** **SUBJECT CARD**	
Name in Polish	
Name in English	**Terrestrial ecology**
Main field of study (if applicable)	**Biotechnology**
Specialization (if applicable)	**Bioinformatics**
Level and form of studies:	**2nd level**
Kind of subject	**obligatory**
Subject code	**OSC024002**
Group of courses	**NO**

*delete as applicable

	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	Examination				
For group of courses mark (X) final course					
Number of ECTS points	3				
including number of ECTS points for practical (P) classes					

including number of ECTS points for direct teacher-student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[45] General knowledge about principles of ecology
[46] General knowledge about natural resources
[47] General knowledge about protection of environment
[48] General knowledge about global climate

SUBJECT OBJECTIVES	
C1	Student should understand the ecological principles
C2	Student should known the aspects of biodiversity
C3	Student should known the natural resources (renewable and nonrenewable)
C4	Student should known the human impact on ecosystem and be familiar with the protection of environment
C5	Student should known the aspects of global climate

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEK_W01 – student knows what terrestrial ecology is

PEK_W02 – student knows the concept of Industrial ecology and Sustainable development

PEK_W03 – student knows the general structure of the Earth, Earth's atmosphere, types of ecological pyramids, Law of tolerance, limiting factors to ecosystem

PEK_W04 – student knows a biome definition, factors that produce biomes, major types and characteristics of terrestrial biomes, biome distribution

PEK_W05 – student knows a classification of aquatic ecosystems, groups of aquatic organisms , characteristics of freshwater and marine ecosystems

PEK_W06 – student knows ecosystem niches, types of ecological interactions and types of ecological succession

PEK_W07 – student knows major mechanisms of evolution, types of biodiversity and ecosystem services

PEK_W08 – student knows characteristics of populations, changes in population size, the form and structure of communities and functional aspects of communities

PEK_W09 – student knows the decomposition processes and major cycles: carbon, nitrogen, phosphorus, sulphur and simplified hydrologic cycle

PEK_W10 – student knows the aspects of food, soil (erosion) and pest management

PEK_W11 – student knows the types of hazardous wastes, aspects of air pollution (primary and secondary air pollutants, the formation of photochemical smog) and water pollution (point and nonpoint sources of water pollution, wastewater treatment)

PEK_W12 – student knows the major types of material resources, types of nonrenewable energy, types of renewable energy

PEK_W13 – student knows the aspects of biomonitoring, types of organisms used in biomonitoring studies

PEK_W14 – student knows the elements of weather and climate, the chemical composition of the atmosphere, structure of the atmosphere, the energy balance in atmosphere, ozone layer, greenhouse effect

PROGRAMME CONTENT		
Form of classes - lecture		Number of hours
Lec 1	Introduction to terrestrial ecology	2
Lec 2	Relevance of biological ecology to industrial ecology	2
Lec 3	Ecosystems. What are they and how do they work	2
Lec 4	Major ecosystems of the world - terrestrial biomes	2
Lec 5	Major aquatic ecosystems of the world	2
Lec 6	Interactions of species in ecosystems; ecological succession	2
Lec 7	Evolution, biodiversity and ecosystem services	2
Lec 8	Population and community ecology	2
Lec 9	Decomposition processes and biogeochemical cycles in ecosystems	2
Lec 10	Food, soil and pest management	2
Lec 11	Human impact on ecosystems	2
Lec 12	Energy for human use	2
Lec 13	Biomonitoring	2

Lec 14	The global climate The energy balance in atmosphere	4
	Total hours	**30**

TEACHING TOOLS USED	
N1	Lecture with the multimedia presentation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
C	PEK_W01- PEK_W14	Exam

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[23] T.E. Graedel, B.R. Allenby, **Industrial Ecology and Sustainable Engineering,** Pearson Education Inc., Boston, 2002.
[24] Egbert Boeker i Rienk van Grondelle, **Environmental Physics,** Wiley, Chichester, 1999.
[25] E. J. Kormondy, **Concepts of Ecology**, Prentice Hall, Upper Saddle River, 1996.
[26] Clint Baird, **Environmental Chemistry**, W.H. Freeman and Co., New York 1995.
[27] G. Tyler Miller Jr., **Living in the Environment,** Wadswards Publishing Company, Belmont, 1992.
[28] Archie W. Culp Jr, **Principles of Energy Conversion**, McGraw-Hill, New York, 1991.

SECONDARY LITERATURE:

[16] Nigel Bunce, **Environmental Chemistry**, Wuerz publishing Ltd., Winnipeg, Canada 1991.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)
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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Terrestrial ecology

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Biotechnology

Subject educational effect	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives***	Programme content***	Teaching tool number***
(knowledge) **PEK_W01**		C1	Lec 1	N1
PEK_W02		C1	Lec 2	N1
PEK_W03		C1	Lec 3	N1
PEK_W04		C1	Lec 4	N1
PEK_W05		C1	Lec 5	N1
PEK_W06		C1	Lec 6	N1
PEK_W07		C2	Lec 7	N1
PEK_W08		C2	Lec 8	N1
PEK_W09		C3	Lec 9	N1
PEK_W010		C3	Lec 10	N1
PEK_W011		C4	Lec 11	N1
PEK_W012		C3, C4	Lec 12	N1
PEK_W013		C4	Lec 13	N1
PEK_W014		C5	Lec 14	N1

Wrocław University of Technology

FACULTY OF CHEMISTRY

SUBJECT CARD

Name in Polish	**Chemia Teoretyczna**
Name in English	**Theoretical Chemistry**
Main field of study (if applicable)	**Chemistry**
Specialization (if applicable)	
Level and form of studies:	**2nd**
Kind of subject	**obligatory**
Subject code	**CHC024040**
Group of courses	**NO**

*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30	15	30		
Number of hours of total student workload (CNPS)	120	30	60		
Form of crediting	Examination	crediting with grade	crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	4	1	2		
including number of ECTS points for practical (P) classes		1	2		
including number of ECTS points for direct teacher-	1	0.5	1		

student contact (BK) classes					

*delete as applicable

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES
[49] General Chemistry, Physics I and II
[50] Algebra, Mathematical Analysis
[51] Ohysical Chemistry, Introduction to Quantum-Chemistry

SUBJECT OBJECTIVES	
C1	Introduction to basic concepts of atoms and molecules.
C2	The skills for predicting structure of molecular systems basing on quantum-chemical methods.
C3	The theoretical interpretation of thermodynamical and electronic properties of molecules and ions.
C4	The ability to make molecular modeling.

SUBJECT EDUCATIONAL EFFECTS

Relating to knowledge:

PEK_W01 – the understanding of problems and shortcomings of classical physics in the microscopic description,

PEK_W02 – the knowledge of quantum mechanical postulates and elements of operator mathematics,

PEK_W03 – the ability to construct of Schrödinger equation (SE) for selected physical problems and for any molecular system,

PEK_W04 – the understanding of SE for hydrogen atom and the interpretation of equation solution,

PEK_W05 – the understanding of atomic structure,

PEK_W06 – the basic knowledge of molecular orbital theory,

PEK_W07 – the understanding of the theory of hybrid orbitals, mesomeric concept, and the idea of multi-center bonds,

PEK_W08 – the knowledge of procedures to solve Hartree-Fock equations and the correlation energy,

PEK_W09 – the understanding of molecular interactions.

Relating to skills:

PEK_U01 – is able to practical apply data from periodic system of elements,

PEK_U02 – knows the interpretation of electronic spectra of hydrogen atom and heavy atoms,

PEK_U03 – the ability to predict molecular structure of organic and inorganic molecules,

PEK_U04 – the ability to interpret of spectroscopic data with regard to quantum-chemical calculations,

PEK_UO5 – the ability to study chemical reaction mechanisms.

PROGRAMME CONTENT		
Form of classes - lecture		Number of hours
Lec 1	**Classical and quantum mechanics**. Mathematical bases of probability theory. Experimental base for wave-corpuscular dualism. The development of quantum concept with elements of Bohr theory and reasons for its collapse.	2
Lec 2	**The foundations of quantum mechanics**. Postulates of quantum mechanics. The definition of wavefunction and its probabilistic interpretation. The definition of operators representing observables.	2
Lec 3	**The foundations of quantum mechanics II**. Schrödinger equation. Eigenvalues and eigenfunctions of Schrödinger equation. Mean values of observables. Properties of eigenfunctions in the case of Schrödinger equation without time.	2
Lec 4	**Hydrogen atom**. Schrödinger equation for hydrogen and hydrogen-like cations. The solution with regard energies and wavefunction. Geometric properties of hydrogen-like orbitals. Quantum numbers. Energy levels and emission spectra of hydrogen.	2

Lec 5	**Pauli exclusion.** Electron spin. Multiplicity of many-electron system. Electronic states of atoms (atomic terms). Fermions and bosons. The concept of spinorbital. Pauli exclusion principle. Slater determinant. Electronic configuration. The structure of periodic system of elements. Hundt's rules.	2
Lec 6	**Many-electron atom.** Hamiltonian and Schrödinger equation for many-electron atom. Slater determinant. Wavefunctions for many electron atoms. Single-electron approximation – spinorbitals and orbitals. Pauli exclusion principle as an antysymmetric function.	2
Lec 7	**Hartree-Fock equations.** The energy expression in single electron approximation. The derivation of Hartree-Fock equations. One and two electron integrals. Exchange energy. Closed and open-shell electronic configuration. The selection rules for optical transition.	2
Lec 8	**Molecule.** Born-Oppenheimer approximation. Schrödinger equation for molecules. Molecular orbital theory. Linear combination of molecular orbitals concept. Hartree-Fock-Roothaan-Hall equations. Thae atomic basis set. Slater and Gaussian functions.	2
Lec 9	**Chemical bond.** Electrostatic and covalent character of chemical bonds. Type of bonds. Orbitals σ and π. Bonding, antybonding, and nonbonding orbitals – energies and geometrical representation. The electronic structure of diatomic molecules. The bond order.	2
Lec 10	**Localized orbitals.** Hybridization sp^3, sp^2 and sp. The representation of electronic density in molecules. Localized orbitals as a tool for the structure prediction. The molecular structure of moieties including phosphorous. The concept of mesomeric representation. Multicenter bonds.	2
Lec 11	**Molecular spectroscopy I.** The rotation and vibration separation. Rotational spectra of diatomic molecules and elements of microwave spectroscopy. The selection rules.	2
Lec 12	**Molecular spectroscopy II.** Vibarational spectra of diatomic and many-atoms molecules. IR and Raman spectra. The selection rules.	2
Lec 13	**Molecular properties based on energy.** Ionization energy, electron affinity. Thermodynamics of chemical processes. Mass spectrometry. The transition state theory. Reaction mechanism.	2
Lec 14	**Properties of molecules based on wavefunction.** Electronic density in the molecule. The bond order. Charge distribution in molecules. Dipole and higher moments in molecules.	2
Lec 15	**Molecular interactions.** The theory of molecular interactions. Electrostatic, exchange, induction, dispersion interactions. Charge-transfer complexes. Hydrogen bond. The second order structure of molecular complexes. Conformational analysis.	2
	Total hours	**30**

Form of classes - class		Number of hours
Cl 1	Organization of classes. Problems with experiment interpretation in classical mechanics and the Born of quantum theory.	2
Cl 2	Operator mathematics. The properties of operators. The Schrödinger equation.	2
Cl 3	The solution of simple quantum mechanical problems: potential well and particle in the box. Related chemical problems. Rotor and oscillator models. The elements of spectroscopy.	2
Cl 4	Hydrogen-like orbitals. Space properties of s, p, d orbitals. Unitary transformation of orbitals. The radial and angular picture of orbitals.The studies of untysymmetric properties of function.	2
Cl 5	Hybridization model. The prediction of molecular structure.	2
Cl 6	Energetical and electronic properties of molecules.	2
Cl 7	Calculations of molecular interactions. Atonic charge distribution. Dipole moment and polarizability.	2
Cl 8	Review and Test.	1
	Total hours	**15**

Form of classes - laboratory		**Liczba godzin**
La1	The local lab and the computing center organization. Accounts distribution and basic information about systems.	2
La2	Elements of UNIX (commends).	2
La3	Elements of UNIX (editors).	2
La4	Gaussian-90 program structure. Execution of the program.	2
La5	The structure representation, matrix-Z.	2
La6	The Hartree-Fock calculations. The output file structure.	2
La7	Molecular graphics program – Molden.	2

La8	Structure optimizations.	2
La9	Frequencies, thermochemistry, and vibrational spectra.	2
La10	Project I – structure and properties of molecule.	2
La11	Energetics of chemical reaction.	2
La12	Project II – frequency calculations, spectra simulation.	2
La13	Heat of reaction, synthesis reaction, atomic charge distribution.	2
La14	Project III – the reaction mechanism.	2
La15	Transition state. Molecular interactions.	2
	Total houres	**30**

TEACHING TOOLS USED	
N1	Lecture
N2	Problems solving
N3	Project preparation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
C	PEK_Lec01- PEK_Lec15	Final exam
F1	PEK_Cl01- PEK_Cl08	Electronic test

F2	PEK_La1- PEK_La15	Projects

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[29] W. Kołos, J. Sadlej, Atom i Cząsteczka, WNT, Warszawa, 1998.
[30] Mechanika Kwantowa dla Chemików, D. O. Hayward, PWN, Warszawa, 2007.
[31] M. A. Ratner, G. C. Schatz, Introduction to Quantum Mechanics in Chemistry, Prentience Hall, Upper Saddle River, 2001.
[32] Gausisian-90 – Electronic manual.

SECONDARY LITERATURE:

[17] L. Piela, Idee Chemii Kwantowej, PWN, Warszawa, 2010.
[18] W. Kołos, Chemia Kwantowa, PWN, Warszawa, 1975.
[19] K. Pigoń, Z. Ruziewicz, Chemia Fizyczna (cz. 2), PWN, Warszawa, 2005.
[20] System elektronicznych korepetycji (e – learning).

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MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Theoretical Chemistry

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Chemistry

Subject educational effects	Correlation between subject educational effect and educational effects defined for main field of study and specialization (if applicable)**	Subject objectives ***	Programme content***	Teaching too number***
(knowladge) PEK_W01	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C1	Wy1	N1
PEK_W02	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C1	Wy3, Wy4	N1
PEK_W03	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C2	Wy2	N1
PEK_W04	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C2	Wy5 – Wy9	N1
PEK_W05	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C3	Wy10	N1
PEK_W06	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C3	Wy11	N1
PEK_W07	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C3	Wy12 – Wy14	N1
PEK_W08	K2Ach_W02, K2Ach_W03, S2Ach1_W06, S2Ach4_W06	C2	Wy15	N1
(skills) PEK_U01	K2Ach_U01, K2Ach_U02, S2Ach2_U05,S2Ach3_ U05	C4	Ćw1 – Ćw3 La6 - La14	N2, N3
PEK_U02	K2Ach_U01, K2Ach_U02, S2Ach2_U05,S2Ach3_ U05	C4	Ćw3 – Ćw7 La6 - La14	N2, N3
PEK_U03	K2Ach_U01, K2Ach_U02, S2Ach2_U05,S2Ach3_ U05	C4	Ćw1 – Ćw5 La6 - La14	N2, N3
PEK_U04	K2Ach_U01, K2Ach_U02, S2Ach2_U05,S2Ach3_ U05	C4	Ćw7 La6 - La14	N2, N3
PEK_U05	K2Ach_U01, K2Ach_U02, S2Ach2_U05,S2Ach3_ U05	C4	Ćw7 La6 - La14	N2, N3

** - enter symbols for main-field-of-study/specialization educational effects

*** - from table above