Analytical Methods in Drug Design and Technology	2
Combinatorial chemistry	7
Crystallography1	1
Graduate laboratory I 1'	7
Graduate laboratory II	0
Graduation seminar and thesis preparation2	3
Inorganic drugs	6
Instrumental drug analysis	0
Mathematical methods in the design and analysis of the experiment	4
Medicinal Natural Products	8
Molecular modeling	4
Multistep Organic Synthesis	9
Philosophy of science and technology	2
Physical organic chemistry	6
Principles of Physiological Chemistry	0
Polymers in medicine	3
Rational drug design	9
Retrieval of scientific and technical information72	3
Selected reactions in organic chemistry7	7
Spectroscopy	1
Synthetic Organic Drugs	6
Theoretical Chemistry	1

# SUBJECT CARD

Name in Polish	Zastosowanie Metod Analitycznych w
	Projektowaniu i Technologii Wytwarzania Leków
Name in English	Analytical Methods in Drug Design and
	Technology
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	Medicinal Chemistry
Level and form of studies:	2nd level, full-time
Kind of subject	obligatory
Subject code	CHC024054
Group of courses	YES

\*delete as applicable

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

\*delete as applicable

#### PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

- 1. Principles of organic chemistry, theoretical and practical.
- 2. Basic knowledge on chromatographic and spectroscopic methods.
- 3. Knowledge in the field of basis of analytical chemistry is recommended.

	SUBJECT OBJECTIVES		
C1	Application of Good Laboratory Practice and validation procedures in analytical		
	methods.		
C2	Gaining of the knowledge on the modern chromatographic techniques and their		
	applications in drug design and technological process of drugs production.		
C3	Acquaintance with the different technological concepts of application of		
	spectroscopic methods in drugs design and quality control in the production system.		
C4	Expanding the knowledge in the field of electrochemical methods applications in the		
	design of biologically active compounds and the production procedures of them.		
C5	Acquaintance with the different concepts in the field of mixed analytical methods		

#### SUBJECT EDUCATIONAL EFFECTS

#### **Relating to knowledge:**

Student, who has completed the course:

- PEK\_W01 has knowledge on the Good Laboratory Practice rules and validation procedures necessary to be used in analytical methods,
- PEK\_W02 has knowledge on the modern chromatographic, spectroscopic, electrochemical and mixed analytical techniques and their applications in drug design and technological process of drugs production,
- PEK\_W03 can define the advantages and disadvantages of the analytical techniques, the sensitivity level of each of them.

#### **Relating to skills:**

Student, who has completed the course:

- PEK\_U01 has skills of use liquid chromatography technique and thin layer chromatography method for separation of a mixture of different compounds, to detect them, do interpretation of the results and prepare the report according to GLP,
- PEK\_U02 has knowledge how to use HPLC system, how to prepare the sample, and how to do the analysis of a mixture of compounds, how to do qualitative and quantitative analysis of them, do interpretation of the results and prepare the report according to GLP,
- PEK\_U03 has knowledge about using different types of mass spectrometry instruments, and about the parameters of the sample ready to analyze,
- PEK\_U04 has skills to do the analysis of a mixture compounds using gas chromatography system, to do interpretation of the results and to prepare the report according to GLP,
- PEK\_U05 has skills to do the analysis of the biologically active compounds using electrochemical methods, do interpretation of the results and prepare the report according to GLP,
- PEK\_U06 has skills to detect the biologically active compounds in a drug formulation using UV-Vis methodology, to prepare a sample, also to control their synthesis following by the kinetic parameters of the reaction,
- PEK\_U07 has knowledge how to estimate the rheological parameters of the drug formulation using viscosimetric technique, to prepare the sample,
- PEK\_U08 has skills to use multiplates reader for turbidimetric measurements, do interpretation of the results and prepare the report according to GLP.

	PROGRAMME CONTENT		
	Form of classes - lecture Number of hours		
Lec 1	Introduction to analytical techniques as tools for drug design and		
	production. Good Laboratory Practice rules in analytical chemistry.	2	
	Pharmacopoeias. Drugs production normalization rules.		
Lec 2	Error estimation in analytical methods used in drugs design and	2	
	technology. Validation techniques.	2	

Lec 3	Chromatographic techniques in drugs design and control of production process.	2
Lec 4	Mixed advanced analytical techniques as a tool in drugs design and control of their activity.	2
Lec 5	Immunoenzymatic assays in design and technology of drugs.	1
Lec 6	6 Mass spectrometry - principles of the method, types of ionization, comparison of used types of analyzers. Principles of fragmentation, application of the method in the investigation of macromolecules structure.	
Lec 7	Potentiometry and conductometry as modern analytical methods.	2
Lec 8	Voltamperometry and other electrochemical methods in drug design and technology.	2
	Total hours	15

	Form of classes - laboratory	Number of hours	
Lab 1	Safety rules in the laboratory of organic chemistry, good laboratory practice and the rules of the reports preparation.	4	
Lab 2	b 2 Liquid chromatography – the separation technique useful in pigments separation. TLC method as a tool of quality control procedure.		
Lab 3	HPLC technique – a scheme of the procedure of a sample preparation. Gripex – isolation of three biologically active compounds – preparation of a sample to HPLC analysis.	4	
Lab 4	HPLC – the equipment scheme. The analysis of Gripex biologically active components.	4	
Lab 5	Scheme of mass spectrometer, types of ionization sources and analyzers. Training in principles of fragmentation.	4	
Lab 6			
Lab 7	Lab 7GC equipment and the procedure of analysis. Application of MS as the detection technique. Separation and identification of the perfume mixture components.		
Lab 8			
Lab 9			
Lab 10			
Lab 11			
Lab 12			

Lab 13	UV-Vis method as the tool to control of kinetic of a reaction. Control technique of synthesis of the biologically active compound.	
Lab 14	Turbidimetry – the analytical method useful to drug design and quality control of it. Control of silver salts formation using microplates reader.	4
Lab 15	Repeating of the not successful realized experiments. Consultation of the reports results.	4
	Total hours	60

	TEACHING TOOLS USED	
N1	N1 Lecture with multimedial presentation.	
N2	N2 Experiment realizing.	
N3	N3 Report preparation.	

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT			
EvaluationEducational effectF - forming (during semester),numberP - concluding (at semester end)		Way of evaluating educational effect achievement	
P1	PEK_W01-W04	Average note of 11 grades of 11 short tests verifying student's knowledge.	
P2 (laboratory)	PEK_U01 – U05	Average note of 10 grades of 10 completed reports, containing result, calculations and conclusions, prepared according to good laboratory practice rules.	

#### PRIMARY AND SECONDARY LITERATURE

#### **PRIMARY LITERATURE:**

- [1] J. Ermer, J.H.McB. Miller, Method Validation in Pharmaceutical Analysis. A Guide to Best Practice. Wiley-VCH, Weincheim. 2005.
- [2] Farmakopea Polska V, Urząd Rejestracji Leków, Wyrobów Medycznych I Produktów Biobójczych, Warszawa, 1990.
- [3] W. Jennings, E. Mittlefehldt, P. Stremple, Analytical Gas Chromatography. 2<sup>nd</sup> Ed. Academic Press, 1997.
- [4] R.P.W. Scott, Tandem Techniques. John Wiley & Sons, 1997.
- [5] M.S. Lee, Integrated Strategies in Drug Discovery Using Mass Spectrometry. John Wiley & Sons, 2005.
- [6] A.J. Bard, R.L. Faulkner, Electrochemical Methods. Fundamental and Applications. John Wiley & Sons, 2001.

#### **SECONDARY LITERATURE:**

- [1] D.M. Bliesner, Validating Chromatographic Methods. A Practical Guide. John Wiley & Sons, 2006.
- [2] P.A. Christensenand A. Hamnett, Techniques and Mechanisms in Electrochemistry. Kluver Academic Press, 1994.
- [3] AC Moffat, MD Osselton, B Widdop, Clarke's analysis of drugs and poisons. Pharmaceutical Press, 2005.
- [4] F.A. Settle, Handbook of Instrumental Techniques for Analytical Chemistry. Prentice-Hall Inc., 1997.

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

Izabela Pawlaczyk, izabela.pawlaczyk@pwr.wroc.pl

# MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Analytical Methods in Drug Design and Technology

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

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 content***	Teaching tool number***
PEK_W01	S2Ach4_W08	C1	Lec1 – Lec8	N1
PEK_W02	S2Ach4_W08	C1, C2, C3, C4, C5	Lec3 – Lec8	N1
PEK_W03	S2Ach4_W08	C1, C2, C3, C4, C5	Lec2 – Lec8	N1
PEK_U01	S2Ach4_U07	C1, C2	Lab1, <b>Lab2</b> , Lab15	N2, N3
PEK_U02	S2Ach4_U07	C1, C2, C3, C5	Lab1, <b>Lab3,</b> <b>Lab4</b> , Lab15	N2, N3
PEK_U03	S2Ach4_U07	C1, C3	Lab1, <b>Lab5,</b> <b>Lab6</b> , Lab7, Lab15	N1, N2, N3
PEK_U04	S2Ach4_U07	C1, C2, C3, C5	Lab1, Lab5, <b>Lab7</b> , Lab15	N2, N3
PEK_U05	S2Ach4_U07	C1, C4	Lab1, <b>Lab8,</b> <b>Lab9, Lab10</b> , Lab15	N2, N3
PEK_U06	S2Ach4_U07	C1, C3	Lab1, <b>Lab12,</b> <b>Lab13</b> , Lab15	N2, N3
PEK_U07	S2Ach4_U07	C1, C5	Lab1, <b>Lab11</b> , Lab15	N2, N3
PEK_U08	S2Ach4_U07	C1, C3, C5	Lab1, Lab12, <b>Lab14</b> , Lab15	N2, N3

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

# **SUBJECT CARD**

Name in Polish	Chemia kombinatoryczna
Name in English	Combinatorial chemistry
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	Medicinal Chemistry
Level and form of studies:	2nd level, full-time
Kind of subject	optional
Subject code	CHC020017
Group of courses	NO
*delete as applicable	

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of					
organized classes in	30				
University (ZZU)					
Number of hours of total	60				
student workload (CNPS)	00				
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-	0.5				
student contact (BK) classes					

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

4. Knowledge of chemistry corresponding to the BSc degree at the Faculty of Chemistry.

	SUBJECT OBJECTIVES		
C1	Knowledge of modern techniques and methods of synthesis of organic compounds		
	libraries in solution and on a solid support.		
C2	Examples of their application in the development of compounds of the targeted		
	biological activity or physicochemical properties		
C3	Presentation of combinatorial synthetic methodologies leading to low molecular		
	weight compounds and natural oligomers.		

#### SUBJECT EDUCATIONAL EFFECTS Relating to knowledge: The person who completed the course: PEK\_W01 – knows the basic theory on the construction and the use of solid polymer supports, understands the role and advantages of immobilization, PEK\_W02 – knows methodologies of obtaining and deconvolution of chemical libraries in solution and on a solid support, PEK\_W03 – got to known examples of combinatorial chemistry application in the development of a product of targeted physicochemical properties, PEK\_W04 – understands the role of combinatorial synthesis in the development of new drugs, PEK\_W05 – is familiar with traditional and combinatorial synthesis of peptides, oligonucleotides, and oligosaccharides,

PEK\_W06 – got to known instrumental techniques of combinatorial chemistry used in the synthesis and analysis of the products.

PROGRAMME CONTENT		
	Form of classes - lecture	Number of hours
Lec 1	Introduction to combinatorial chemistry. Basic concepts. Traditional chemistry versus parallel and combinatorial synthesis.	2
Lec 2	Combinatorial libraries in solution. Indexed libraries. Scaffolds.	2
Lec 3	Structure and examples of solid supports. Polymer resins. Merrifield, Wang, Mitchell and Rink resin. Structure and function of linkers and spacers.	2
Lec 4	Strategies for the synthesis of peptides on a solid support. Protecting groups, coupling agents. Advantages of immobilization. Instrumentation and apparatus.	2
Lec 5	Peptide libraries. Preparation by coupling of isokinetic mixtures and "mix and split" method. Examples of application.	2
Lec 6	Libraries of oligonucleotides. Flow synthesis. Microarrays. Phage display.	2
Lec 7	Classical and combinatorial synthesis of oligosaccharides on a solid support. Sugar units as a "scaffold". Soluble solid support.	2
Lec 8	Methods of deconvolution of combinatorial libraries. Isolation of the active component.	2
Lec 9	Determining the structure of the active compound. Instrumental techniques. Tags. Encoded libraries.	2
Lec 10	Organic synthesis on a solid support. Immobilized reagents. Examples of low molecular weight compound libraries.	2
Lec 11	Multicomponent reactions. Isonitriles. Passerini and Ugi condensations.	2
Lec 12	Combinatorial chemistry in drug design.	2
Lec 13	Other applications: catalysis, materials science.	2
Lec 14	Instrumentation of combinatorial chemistry. Automated synthesis.	2
Lec 15	Analytical techniques in the characterization of combinatorial	2

	libraries.	
	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		
С	PEK_W01 - PEK_W06	multimedia presentation		

## PRIMARY AND SECONDARY LITERATURE

# PRIMARY LITERATURE:

- [7] Molecular Diversity and Combinatorial Chemistry: Principle and Applications (M. C. Pirrung Ed.); Elesevier, 2004.
- [8] Combinatorial Chemistry and Technologies: Methods and Applications (G. Fassina, S. Miertus Eds); Taylor and Francis, 2005.
- [9] A. Furka. Combinatorial Chemistry. Principles and Techniques, http://members.iif.hu/furka.arpad/BookPDF.pdf

# **SECONDARY LITERATURE:**

- [1] Combinatorial Chemistry: Synthesis, Analysis, Screening (G. Jung Ed.); Wiley, 2001.
- [2] Combinatorial Chemistry: From Theory to Application (W. Bannwarth, B. Hinzen Eds.); Wiley, 2005.

# SUBJECT SUPERVISOR

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# MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Combinatorial Chemistry

#### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

all fields of Faculty of 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	elective	C1	Lec 1, Lec 3	N1
PEK_W02		C1	Lec 2, Lec 4 – Lec 11	N1
PEK_W03		C2, C3	Lec 5 – Lec 7, Lec 12, Lec 13	N1
PEK_W04		C2, C3	Lec 12	N1
PEK_W05		C2, C3	Lec 4 – Lec 7	N1
PEK_W06		C1	Lec 5, Lec 6, Lec 9, Lec 14, Wy15	N1

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

# SUBJECT CARD

Name in Polish	Krystalografia
Name in English	Crystallography
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	Medicinal chemistry, Chemical metallurgy,
	Organic and polymer chemistry
Level and form of studies:	2nd level, full-time
Kind of subject	obligatory
Subject code	CHC024053
Group of courses	NO
delete as applicable	

Lecture Classes Laboratory Project Seminar Number of hours of organized classes in 30 15 University (ZZU) Number of hours of total 90 60 student workload (CNPS) crediting Examination Examination Examination Examination Form of crediting with grade\* / crediting / crediting / crediting with grade\* with grade\* with grade\* For group of courses mark (X) final course Number of ECTS points 3 2 including number of ECTS 2 points for practical (P) classes 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

5. Knowledge of 1<sup>st</sup> level degree inorganic and organic chemistry.

6. Knowledge of analytical geometry and group theory at a basic level.

	SUBJECT OBJECTIVES		
C1	To provide the students with a basic knowledge of Crystallography.		
C2	To make the students understand the intermolecular interactions in the context of		
	solid state molecular organization.		
C3	To make the students familiar with the crystal systems, symmetry operations as well		
	as with the crystallographic point and space groups.		
C4	To make the students familiar with some basic inorganic crystal structures.		
C5	To make the student s familiar with the basis of the X-ray diffraction measurements		
	and analysis.		
C6	To make the students familiar with Cambridge Structural Data Bases (CSD) and		
	their importance for structural studies		

SUBJECT EDUCATIONAL EFFECTS
Relating to knowledge:
PEK_W01 – The student knows the basic conception of a crystal and a crystal lattice.
PEK_W02 – The student knows the basic intermolecular interactions and understands their
character.
PEK_W03 – The student knows the macroscopic and structural symmetry elements and
operations in the crystal and understands their combinations.
PEK_W04 – The student knows the 32 crystal point groups and understands the crystal space groups.
PEK_W05 – The student knows the basic metallic, covalent and ionic structures.
PEK_W06 – The student knows the X-ray diffraction theory and the basic diffraction equations
PEK_W07 – The student has some knowledge about crystal diffraction measurements and structure solutions.
PEK_W08 – The student has some knowledge about Crystallographic Data Bases.
Relating to skills:
PEK_U01 – The student knows how to use the resources of the Cambridge Structural Database.
PEK_U02 – The student is able to define the Miller indices.
PEK_U03 – The student is able to read the information inhibited in the space group symbol.
PEK_U04 – The student is able to distinguish centrosymmetric, noncenrosymmetric and chiral space groups.
PEK_U05 – The student is able to use the International Tables for Crystallography.
Relating to social competences:
PEK_K01 PEK_K02
_

	PROGRAMME CONTENT		
	Form of classes - lecture	Number of hours	
Lec 1	Introduction to the course of crystallography. Vectors and matrices in crystallography. Coordinate systems in crystallography and crystallographic calculations.	2	
Lec 2	The symmetry: Symmetry elements and symmetry operations. The symmetry of the finite sets.	2	
Lec 3	The crystal lattice theory: primitive and complex networks. Lattice planes and crystal directions: Miller indices and zone axis symbols. The unit cell and the crystal systems. Indexing in trigonal and hexagonal systems.	2	
Lec 4	Two- and three-dimensional lattices and symmetry. The five plane lattices; the seventeen plane groups. One-dimensional symmetry:	2	

...

	Total hours	30
Lec 15	Cambridge Crystallographic Data Base. Analysis of crystal structures	2
Lec 14	Crystal diffraction: Atom displacement factors. Structure factors. Symmetry of the diffraction patterns – the Laue groups, systematic absences	2
Lec 13	Crystal diffraction: X-ray diffraction. The Laue equations. The Bragg's equation; higher order of diffraction; the quadratic form of Bragg equation. The Ewald reflecting sphere construction.	2
Lec 12	Some important ionic structures and covalent structures.	2
Lec 11	Classification of solid state structures: hexagonal layer and close packed crystal structures: hcp, ccp, bcc structures. Octahedral and tetrahedral interstices and their positions in closed packed structures. Atomic radius. Basic metallic structures.	2
Lec 10	Crystal organization and lattice energy. Chemical bonding and intermolecular interactions.	2
Lec 9	The tree-dimensional space groups. International symbols. Interpretation the information from the International Crystallographic Tables.	2
Lec 8	The 17 crystallographic space groups of two-dimensional lattices. Ortogonal projections. General and special positions.	2
Lec 7	Crystal space symmetry: Translational symmetry; screw rotations and glide planes. International symbols.	2
Lec 6	Crystal morphology and geometrical crystal shapes : open and closed crystal shapes. Symmetry of the crystal polyhedrons and symbols of the polyhedron walls.	2
Lec 5	Crystal symmetry. Stereographic projections. Lattice and crystal point symmetry and symmetry elements. The 32 crystallographic point groups. The symmetry classifications of crystal systems.	2
	border or frieze patterns. The fourteen Bravais lattices and the crystal systems. The reciprocal lattice.	

	Form of classes - class	Number of hours
Cl 1	Vectors in crystallography: bases vectors and coordinates; the scalar and the vector product. Matrices in crystallography: matrix operations; matrix transformation; determinant; the inverse of a matrix.	1
Cl 2	Coordinate systems in crystallography. Change of bases. Unit cell basis and orthonormal basis. Identity of vector triple product and scalar triple product.	1
Cl 3	Symmetry operations: Stereographic projections; matrix representation; combined and coupled symmetry operations.	1
Cl 4	Defining the Miller indices of axes and planes. The zone axes symbol.	1
Cl 5	Geometrical calculations. Determining distances and angles in the unit cell. Determining the cell volume.	1
Cl 6	Symmetry classification of crystal systems. The Miller-Bravais symbons in hexagonal system.	1
Cl 7	Combination of symmetry elements. Crystallographic point groups . Point group stereograms. Stereographic projections of the crystal polyhedrons.	1

C1 8	Symmetry of the plane lattices. Two-dimensional space groups. Preparing the orthogonal projections of the 17 plane groups.	1
Cl 9	Symmetry of the three-dimensional lattices. Three-dimensional space groups. Interpretation information of the space group symbol.	1
Cl 10	Close packed structures. Atomic packing factor, volume of the interstices: calculations	1
Cl 11	Two-component structures - calculations	1
Cl 12	Bragg equation. Calculations	1
Cl 13	Systematic absence of reflections. Laue groups.	1
Cl 14 - Cl 15	Crystallographic Data Base Cambridge	2
		15
	Total hours	

	TEACHING TOOLS USED		
N1	Lectures in the Internet.		
N2	Multimedia presentations		
N3	The use of specialized software.		
N4	Troubleshooting tasks		
N5	Consultation		

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 (lectures)	PEK_W01 – PEK_W08	exam			
F1 (exercise)	PEK_U02- PEK_U05	colloquium			
F2 (activity)	PEK_U02- PEK_U05				
C(exercise) = 0.8F1 + 0.2F2					

## PRIMARY AND SECONDARY LITERATURE

#### **PRIMARY LITERATURE:**

- [3] Dennis W. Bennett, Understanding Single-Crystal X-Ray Crystallography, Wiley-VCH, 2010.
- [4] Christopher Hammond, The Basics of Crystallograaphy and Diffraction, 3<sup>rd</sup> Eddition, IUCr, Oxford University Press, 2011.
- [5] Werner Massa, Crystal Structure Determination, Springer, Berlin, 2004.
- [6] J. Glusker and K. Trueblood, Crystal Structure Analysis, Oxford Science Publication, 2010.

#### **SECONDARY LITERATURE:**

- [7] Zygmunt Trzaska Durski i Hanna Trzaska Durska, Podstawy Krystalografii, PANalytical, Warszawa 2003.
- [8] Zygmunt Trzaska Durski i Hanna Trzaska Durska, Podstawy Krystalografii strukturalnej i rentgenografii, PWN, Warszawa, 1994.
- [9] Z. Bojarski, M Gigla, K. Stróż, M. Surowiec, Krystalografia, PWN, Warszawa 1996.
- [10] Z. Bojarski, M Gigla, K. Stróż, M. Surowiec, Krystalografia, PWN, Warszawa 2007.

# SUBJECT SUPERVISOR

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Prof. dr hab. Veneta Videnova-Adrabińska, Veneta@pwr.wroc.pl

## MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Crystallography

#### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

#### 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	K2Ach_W04	C1	Lec 1	N1
PEK_W02	K2Ach_W04	C2	Lec 10 - Lec 12	N1, N2
PEK_W03	K2Ach_W04	C3	Lec 2, Lec 7	N1, N2
PEK_W04	K2Ach_W04	C3	Lec 4, Lec 5, Lec 8	N1, N2
PEK_W05	K2Ach_W04	C2, C4	Lec 11, Lec 12	N1, N2
PEK_W06	K2Ach_W04	C5	Lec 13,	N1, N2
PEK_W07	K2Ach_W04	C5	Lec 14	N1, N2

PEK_W08	K2Ach W04	C6	Lec 15	N1, N2
(skills) PEK_U01	K2Ach_U04	C6	Cl 1-Cl 15	N3
PEK_U02	K2Ach_U04	C3	Cl 3- Cl 5	N2, N4
PEK_U03	K2Ach_U04	C3	Cl 2- Cl 9	N2, N4
PEK_U04	K2Ach_U04	C3, C4	Cl 2- Cl 9	N2, N4
PEK_U05	K2Ach_U04	C1, C3, C5	Cl 9	N2, N4
(competences) PEK_K01				
PEK_K02				
PEK_K03				

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

# **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- student contact (BK) classes			2		

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

7. Theoretical and practical knowledge required for the degree program being studied 8.

	SUBJECT OBJECTIVES			
C1	C1 Get to know the basic methodology of scientific work			
C2	C2 Acquisition of the ability to use the scientific literature and other sources of			
	knowledge.			
C3	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**

	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				
С	PEK_W01 PEK_W02 PEK_U01 – PEK_U03	evaluation of the quantity and quality of student work				

#### PRIMARY AND SECONDARY LITERATURE

[11] 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

# **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			225		
University (ZZU)					
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			7,5		

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

9. Theoretical and practical knowledge required for the degree program being studied 10.

	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				
С	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

[12] 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

# SUBJECT CARD

Name in Polish	<b>Seminarium dyplomowe</b> (+ 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	CHC024001
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 *delete as applicable					0,5

\*delete as applicable

#### PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

#### Theoretical and practical knowledge required for the degree program being studied 11. 12.

	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		
Sem 1-15	Presentation of multimedia presentation and participate in the discussion	15	
	Total hours	15	

TEACHING TOOLS USED			
N1	N1 consultations		
N2	N2 multimedia presentation		
N3	N3 oral presentation		

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

# PRIMARY AND SECONDARY LITERATURE

# **PRIMARY LITERATURE:**

[10] none

# **SECONDARY LITERATURE:**

[13] none

[14]

#### 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

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

Zał. nr 4 do ZW 64/2012

Wrocław University of Technology FACULTY OF CHEMISTRY

Name in Polish:
Name in English:
Main field of study (if applicable):
Specialization (if applicable):
Level and form of studies:
Kind of subject:
Subject code
Group of courses

#### SUBJECT CARD Leki Nieorganiczne Inorganic drugs Chemistry Medicinal Chemistry 2nd level, full-time obligatory CHC024019 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	credit				
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	_				

#### PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Completed courses in Inorganic Chemistry and Organic Chemistry, 1-st level

#### SUBJECT OBJECTIVES

- C1 Learning the fundamental topics and techniques in medicinal chemistry.
- C2 Gaining a knowledge about the modern methods in medical diagnostics (PET, MRI, MRA, SPECT) employing metal compounds and radioisotopes.
- C3 Learning the chemical structures, methods of syntheses ad the mechanisms of action of the inorganic drugs.
- C4 Learning the current trends in the development of inorganic drugs.

#### SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEK\_W01 Student gains a general knowledge about the contemporary diagnostic techniques used in medicine: magnetic resonances (MRI and MRA), positron emission tomography (PET), Single Photon Emission Computed Tomography (SPECT). Knows the metal compounds and radiopharmaceuticals used in these diagnostic techniques.

PEK\_W02 Knows the application of inorganic drugs in the medical therapy.

	Form of classes – lecture	Number of hours
Lec 1	Classification of drugs. Drug targets. Drug discovery, design and development (clinical trials).	2
Lec 2	Development of Inorganic Drugs. The dose-response relationship. Bertrand diagram.	2
Lec 3	Inorganic diagnostic contrast agents. Barium sulfate and iodine compounds as X-ray contrasts. Instrumentation and the basic mechanism of Magnetic Resonance Imaging (MRI). Gadolinium(III) chelates, nanomolecules and iron oxides nanoparticles as T1 and T2 contrast agents in magnetic resonances (MRI and MRA).	2
Lec 4	PET, Positron Emission Tomography. Instrumentation and the basic mechanism. Radiopharmaceuticals containing F-18, O-15, N-13 and C-11 as diagnostic agents. Metal-based PET radiotracers: Cu-64, Rb-82 and Ga-68 labeled compounds. Portable generator for obtaining the positron emitters (instant kit). Application of PET method.	2
Lec 5	Nuclear medicine and the use of radio-nuclides (gamma - emission). Scintigraphy and Single Photon Emission Computerized Tomography (SPECT) in tumor diagnostics. Radionuclide production. Technetium (Tc-99m), gallium (Ga-67) and indium (In-111) - labeled compounds.	2
Lec 6	Therapeutic radiopharmaceuticals: therapy of cancer with radioisotopes. The use of the monoclonal antibodies with gamma-emitters. Samarium (Sm-153) and tin (Sn-117) complexes in bone-pain palliation. Boron- Neutron Capture (BNC) therapy. Structure and functions of DNA – an overview.	2
Lec 7	The origin of cancer. The chemical and physical mutagens. Anti- oncogens, protein p-53, cell apoptosis. Various types of chemotherapy. Drugs acting directly on DNA: alkylating agents (chlormethine); intercalators and chain cutters. Bleomycin and the role of a metal ion.	2
Lec 8	Discovery of Cisplatin. Hydrolysis and kinetics of binding to DNA. Structures of DNA adducts produced by cisplatin. The mechanism of anticancer activity of cisplatin.	2
Lec 9	II-nd and III-rd generation of cisplatin analogs. Structures of Carboplatin, Oxaliplatin, Nedaplatin and Picoplatin. Search for an orally active drug. Pt(II) and Pt(IV) complexes. Syntheses of platinum complexes.	2
Lec 10	Search for non-platinum antitumor metal complexes. Palladium, titanium and group 14 metal compounds. Drugs containing arsenic ion. Anticancer activity of arsenic trioxide (Trisenox) and gallium complexes.	2
Lec 11	Ruthenium complexes for selective treatment of solid tumor metastases. Syntheses and structures of ruthenium complexes. The mechanisms of transport and antitumor action of Ru(III) and Ru(II) complexes.	2
Lec 12	Bismuth in medicine, antiulcer and antibacterial properties. <i>Helicobacter pylori</i> . Mechanism of action of bismuth against <i>H.pylori</i> . Drugs containing sulphur: sulfonamides, penicillins, cephalosporins.	2
Lec 13	Vanadium complexes for diabetes treatment (replacement of insulin injections, insulin mimetics). Inorganic vanadium salts (vanadyl sulfate). Chelated oxovanadium complexes. V-O, V-N and V-S coordination	2

	vanadyl complexes. Peroxovanadates.	
Lec 14	Chrysotherapy. Gold – drug metabolism and immunochemistry. Possible mechanism of chrysotherapy in rheumatoid arthritis. Use of gold for other diseases (antitumor activity).	2
Lec 15	Perspectives in medicinal inorganic chemistry	2
	Total hours	30

# **TEACHING TOOLS USED**

N1. Lectures with multimedia presentations (slides)

EVALUATION	OF SUBJECT EDUCATIO	NAL EFFECTS ACHIEVEMENT
Evaluation (F –	Educational effect number	Way of evaluating educational effect achievement
forming (during		
semester), P –		
concluding (at		
semester end)		
Р	PEK_W01- PEK_W02	Final Examination

## PRIMARY AND SECONDARY LITERATURE

## **PRIMARY LITERATURE:**

[1] G.L. Patrick, An Introduction to Medicinal Chemistry III ed. Oxford Univ. Press, 2005.

[2] Metallopharmaceuticals I, DNA Interactions Eds. M.J. Clarke, P.J. Sadler (1999).

[3] Metallopharmaceuticals II, Diagnosis and Therapy. Eds. M.J. Clarke, P.J. Sadler (1999).

- [4] H.B. Kraatz, N. Metzler-Nolte (Eds.), *Concepts and Models in Bioinorganic Chemistry*, 2006, Part 2. *Medicinal Inorganic Chemistry*, pages 25 46.
- [5] E. Alessio (Ed.) Bioinorganic Medicinal Chemistry, Wiley-VCH, 2011

# SECONDARY LITERATURE:

[1] J.C. Dabrowiak *Metals in Medicine*. Wiley, 2009 (an electronic version available)

[2] J.L.Sessler, S.R.Doctrow, T.J.McMurry, S.J.Lippard, Medicinal Inorganic Chemistry 2005

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

prof. zw. dr hab. inż. Danuta Michalska, danuta.michalska@pwr.wroc.pl

## MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR A SUBJECT Inorganic drugs AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY Chemistry

# AND SPECIALIZATION 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 content***	Teaching tool number***
Relating to knowledge PEK_W01	X2A_W06	C2	Lec 3 – Lec 5, Lec 15	N1
PEK_W02	X2A_W06	C1, C3, C4	Lec1 –Lec2, Lec 6-15	N1

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

# 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:	<del>1st</del> / 2nd* level, <del>full-time / part-time</del> *
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

13. 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	N1 Informative lectures	
N2	N2 Implementation of experiments	
N3	N3 Preparation of reports	
N4	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 (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

(NAME AND SURNAME, E-MAIL ADDRESS)

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

Zał. nr 4 do ZW 33/2012

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
* 1 - 1 - 4 - 4 - 6 4 1 - 4 1	

\*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,	
Les	explicit and implicit scheme: case study using MATLAB	
Le4	Linear regression – least squares method, correlation coefficient,	
LC4	sum of squares, error: case study using MATLAB and Excel	
Le5	Nonlinear regression, linearization, normal equation, Gauss-Newton	2
Les	method: case study using MATAB and Excel.	
Le6	Fitting model, chi-square test, Kolmogorov-Smirnov test, Grubb	2
Leo	test: case study using Origin and MATLAB.	
Le7	Statistical hypothesis testing, normal distribution, t-Student	2
Le/	distribution, ANOVA: case study using Origin and Excel.	
L aQ	Response surface method, Box-Benhken method: case study using	1
Le8	MATLAB.	
	Total hours	15

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

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT				
<b>Evaluation</b> (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 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***
( <b>knowledge</b> ) 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

# SUBJECT CARD

Name in Polish	Naturalne Produkty Medyczne
Name in English	Medicinal Natural Products
Main field of study (if applicable)	Chemistry, Biotechnology
Specialization (if applicable)	Medicinal chemistry, Pharmaceutical
	biotechnology
Level and form of studies:	2nd level, full-time
Kind of subject	obligatory
Subject code	CHC024015
Group of courses	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)	30		60		
Form of crediting	Examination		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

14. General knowledge of organic chemistry

15.

#### SUBJECT OBJECTIVES

C1	General knowledge of herbal primary metabolic buildings blocks
C2	General knowledge of herbal secondary metabolic buildings blocks
C3	Knowledge of biological active herbal compounds
C4	Knowledge concerned the application of biological active compounds
C5	Knowledge of english terminology of natural medicinal compounds
C6	Knowledge of isolation methods and identification techniques of natural compounds

SUBJECT EDUCATIONAL EFFECTS				
Relating to knowledge:				
PEK_W01 – knowledge of basic definitions of phitochemistry, chemistry of natural products				
PEK_W02 – classification of herbal building blocks				
PEK_W03 – basic knowledge of herbal metabolic pathways				
PEK_W04 – basic knowledge of coumarins				
PEK_W05 - basic knowledge of flavonoids and stilbenes				
PEK_W06 - basic knowledge of terpenoids and steroids				
PEK_W07 - basic knowledge of alkaloids and glycosides				
PEK_W08 - basic knowledge of natural anticancer compounds				
PEK_W09 - basic knowledge of english terminology of medicinal natural products				
Relating to skills:				
PEK_U01 – knowledge of basic rules of work in laboratory of organic chemistry				
PEK_U02 – practical knowledge of methods of isolation of natural product from herbal material				
PEK_U03 – practical knowledge of methods of distillation and extraction in processes of				
isolation of natural product				
PEK_U04 – practical knowledge of methods of chromatography in identification and				
purification of natural product				
PEK_U05 – practical knowledge of determining of acidic and ester number				
Relating to social competences:				
PEK_K01				
PEK_K02				

	PROGRAMME CONTENT				
	Form of classes - lecture	Number of hours			
Lec 1	<b>Development of phytochemistry and chemistry of natural</b> <b>products.</b> The lecture concerns the history of using of biological active substances in curing different types of diseases.	1h/			
Lec 2- 3	<b>Herbal biological active compounds.</b> Interest has revived recently in the investigation of medicinal plants to identify novel active phytochemicals that might lead to drug development. Nature has generated such substances for millennia — before modern synthetic chemistry. Because these substances arise from a more or less hostile environment, the percentage of biologically active natural substances is relatively high in comparison with substances from artificial sources. Currently more than 50% of drugs in clinical use have a natural-product origin.	2h			
Lec 4- 5	<b>Herbal building blocks.</b> Metabolites are compounds synthesized by plants for both essential functions, such as growth and development (primary metabolites), and specific functions, such as pollinator attraction or defense against herbivory (secondary metabolites). Secondary metabolites are often colored, fragrant, or flavorful compounds, and they typically mediate the interaction of plants with	2h			

	-	
	other organisms. Such interactions include those of plant-pollinator, plant-pathogen, and plant-herbivore. Because of the importance of these and other primary pathways in enabling a plant to synthesize, assimilate, and degrade organic compounds, primary metabolites are essential.	
Lec 6- 7	<b>Coumarins.</b> They belong to the benzopyrones family and possess a wide range of pharmaceutical applications including cytoprotective and modulatory functions, which may be translated into therapeutic potential for multiple diseases. Several natural and synthetic coumarins and derivatives, such as coumarin glycosides, possess potent biological activities. Coumarin derivatives are found in antibiotic, antimitotic, immunomodulating, antiviral, anticancer, anti-inflammatory, anticoagulant, antifungal, antioxidant, and cytotoxic agents, as well as some biological assays.	2h
Lec 8- 9	<b>Flavonoids and stilbenes.</b> Polyphenolic compounds that are ubiquitous in nature and are categorized, according to chemical structure, into flavonols, flavones, flavanones, isoflavones, catechins, anthocyanidins and chalcones. Over 4,000 flavonoids have been identified, many of which occur in fruits, vegetables and beverages (tea, coffee, beer, wine and fruit drinks). The flavonoids have aroused considerable interest recently because of their potential beneficial effects on human health-they have been reported to have antiviral, anti-allergic, antiplatelet, anti-inflammatory, antitumor and antioxidant activities. Stilbenes are a small family of plant secondary metabolites derived from the phenylpropanoid pathway, and produced in a number of unrelated plant species. These compounds have numerous implications in plant disease resistance and human health.	2h
Lec 10-13	<b>Terpenoids and steroids.</b> Terpenoids or isoprenoids, a subclass of the prenyllipids (terpenes, prenylquinones, and sterols), represent the oldest group of small molecular products synthesized by plants and are probably the most widespread group of natural products. Terpenoids can be described as modified terpenes, where methyl groups are moved or removed, or oxygen atoms added. They are universally present in small amounts in living organisms, where they play numerous vital roles in plant physiology as well as important functions in all cellular membranes. A steroid is a type of organic compound that contains a characteristic arrangement of four cycloalkane rings that are joined to each other. Examples of steroids include the dietary fat cholesterol, the sex hormones estradiol and testosterone and the anti-inflammatory drug dexamethasone.	4h
Lec 14-15	Alcaloids and glycosides. Alkaloids are compounds containing nitrogen in a heterocyclic ring that are common to about 15 to 20% of all vascular plants. They are synthesized by plants from amino acids. Alkaloids are subclassified on the basis of the chemical type of their nitrogen containing ring. Alkaloids are formed as metabolic by- products. However, their characteristic bitter taste and accompanying toxicity generally help to repel insects and herbivores. Glycosides play numerous important roles in living organisms. Many plants store	2h

chemicals in the form of inactive glycosides. These can be activated by enzyme hydrolysis, which causes the sugar part to be broken off, making the chemical available for use. Many such plant glycosides	
are used as medications. In animals and humans, poisons are often bound to sugar molecules as part of their elimination from the body.	
Total hours	15h

	Number of hours	
Lab 1	Organizatinal class and lab safety rules	2
Lab 2-3	Alkaloids of pepper. Isolation of piperidine from pepper. TLC as identification method.	4
Lab 4-5	Herbal fats – isolation of trimyristin from nutmeg. Determination of ester number.	4
Lab 6-7	Hydrolysis of trimyristin. Determination of acidic number. I Test	4
Lab 8-9	Steroids – cholesterol of hen egg.	4
Lab 10-11	Licopene and beta-carotene - isolation of products of tomato or carrot. Column chromatography.	4
Lab 12-13	Triterpenes. Isolation of betulin from birch bark. Continuous extraction.	4
Lab 14-15	Isolation of eugenol of gloves. II Test.	4
	Total hours	30

TEACHING TOOLS USED			
N1	N1 Lecture with multimedia presentation		
N2	N2 Laboratory – experimental work		
N3	N3 Laboratory - report		

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT					
Evaluation	Educational effect	Way of evaluating educational effect			
F – forming (during	number	achievement			
semester),					
C – concluding (at					
semester end)					
F1 (lecture)	PEK_W01 -	exam			
	PEK_W09				
F2 (laboratory)	PEK_U01 -	Test I (max 8 points)			
	PEK_U03	_			
F3 (laboratory)	PEK_U03 -	Test II (max 8 points)			
	PEK_U05				
F4 (laboratory)	PEK_U01 -	Correctness of experimental work and			
	PEK_U05	preparation of reports (max 8 points)			
<b>C</b> (laboratory) = $3.0$ when $(F2 + F3 + F4) = 16.0 - 17.5$ pkt.					
3.5  when  (F2 + F3 + F4) = 18.0 - 19.0  pkt.					
4.0 when $(F2 + F3 + F4) = 19.5 - 20.5$ pkt.					
4.5 when $(F2 + F3 + F4) = 21.0 - 22.5$ pkt.					

5.0 when (F2 + F3 + F4) = 22.5 - 23.5 pkt. 5.5 when (F2 + F3 + F4) = 24.0 pkt.

#### PRIMARY AND SECONDARY LITERATURE

#### **PRIMARY LITERATURE:**

[11] P.M. Dewick, *Medicinal natural products*, Wiley 2009

[12] J. Sołoducho, J. Cabaj, *Medicinal natural products – lecture*, PRINTPAP Łódź, 2011

[13] J. Sołoducho, J. Cabaj, *Medicinal natural products – laboratory*, elektronic materials

#### **SECONDARY LITERATURE:**

[15]

[16]

[17]

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

Prof. dr hab. Jadwiga Sołoducho, Jadwiga.soloducho@pwr.wroc.pl

## MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Medicinal Natural Products

#### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

Chemistry/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	S2Ach4_W02	C3-C5	L1-L2	N1		
PEK_W02	S2Ach4_W02	C1-C2, C5	L 3-L4	N1		
PEK_W03	S2Ach4_W02	C1-C2, C5	L5	N1		
PEK_W04	S2Ach4_W02	C3, C5	L6-L7	N1		
PEK_W05	S2Ach4_W02	C3, C5	L8-L9	N1		
PEK_W06	S2Ach4_W02	C3, C5	L10-L13	N1		
PEK_W07	S2Ach4_W02	C3, C5	L14-L15	N1		
PEK_W08	S2Ach4_W02	C4, C5	L2	N1		
PEK_W09	S2Ach4_W02	C5	L1-L15	N1		
(skills) PEK_U01	S2Ach4_W02	C5, C6	Lab1	N2, N3		
PEK_U02	S2Ach4_W02	C5, C6	Lab2-15	N2, N3		
PEK_U03	S2Ach4_W02	C5, C6	Lab2-15	N2, N3		
PEK_U04	S2Ach4_W02	C5, C6	Lab2-3; Lab10- 11	N2, N3		

PEK_U05	S2Ach4_W02	C5, C6	Lab4-7	
(competences) PEK_K01	S2Ach4_W02	C5	L1-L15	N1
PEK_K02	S2Ach4_U02	C5-C6	Lab1	N2, N3
PEK_K03	S2Ach4_U02	C5-C6	Lab2-Lab15	N2, N3
•••	S2Ach4_U02	C5-C6	Lab2-Lab15	N2, N3

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

## **SUBJECT CARD**

Name in Polish	Modelowanie molekularne
Name in English	Molecular modeling
Main field of study (if applicable)	Biotechnology
Specialization (if applicable)	<b>Bioinformatics, Medicinal Chemistry</b>
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- student contact (BK) classes	2		1		1

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

- 16. Basic knowledge of atomic and molecular structure concepts
- 17. Basic knowledge of analytic geometry
- 18. Basic knowledge of computer science
- 19. 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

#### **Relating to knowledge:**

PEK_W01 - knowledge of	construction of 3-dimensional molecular models and the	eir
transformation	S	

- 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			
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
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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		
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	Educational effect	Way of evaluating educational effect
F – forming (during	number	achievement

semester),		
C - concluding (at a consistent and)		
semester end)	DEV 1101	Tast #1
F1 (lecture)	PEK_U01	Test #1
F2 (lecture)	PEK_U02	Test #2
	PEK_U03	
C (lecture) = $F1 + F2$	·	
C (seminar)	PEK_W01	Student multimedia presentation
	PEK_W02	
	PEK_W03	
	PEK_W04	
F3 (lab)	PEK_U05	Partial report #1
F4 (lab)	PEK_U01	Partial report #2
	PEK_U02	
F5 (lab)	PEK_U02	Partial report #3
	PEK_U03	
F6 (lab)	PEK_U04	Partial report #4
C (lab) = F3 + F4 + F5 + F3 + F4 + F5 + F3 + F4 + F5 + F5 + F4 + F5 + F5 + F5 + F5	- F6	

#### **PRIMARY LITERATURE:**

- [14] L. Piela, Quantum Chemistry Ideas, Elsevier, 2010
- [15] A.R. Leach, Molecular Modeling:Principles and Applications, 2 wydanie, Prentice Hall, 2001
- [16] H.D. Hotje, Molecular modeling. Basic principles and applications, 3 wydanie, Wiley, 2008
- [17] T. Schlick, Molecular modeling and simulation, Springer, 2002.

#### **SECONDARY LITERATURE:**

- [18] F. Jensen, Introduction to computational chemistry, Wiley, 2006 (2-nd Ed)
- [19] J.M. Goodman, Chemical Applications of Molecular Modeling, RSC, 1999.
- [20] J.P. Doucet, J. Weber, Computer-Aided Molecular Design, 1996, Academic Press, 1996
- [21] 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 <b>X2A_W02 X2A_W03</b>	C2	Wy2,Wy6 Se3, Se4	N1,N2, N4
PEK_W03	T2A_W02 T2A_W03 <b>X2A_W02 X2A_W03</b>	C3	Wy4, Wy6 Se5, Se6	N1,N2, N4
PEK_W04	T2A_W02 T2A_W03 <b>X2A_W02 X2A_W03</b>	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 <b>X2A_U03 X2A_U04</b> InzA_U01	C4	La3, La4, La5	N3, N5

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

# **SUBJECT CARD**

Name in Polish	Wieloetapowa Synteza Organiczna
Name in English	Multistep Organic Synthesis
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	Medicinal Chemistry
Level and form of studies:	2nd level, full-time
Kind of subject	obligatory
Subject code	CHC024016
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			0.5		

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

20. Knowledge and skills at the level of completion of "Fundamentals of Organic Chemistry - laboratory" course, or equivalent.

#### SUBJECT OBJECTIVES

C1	Gathering proficiency in the laboratory work using advanced experimental
	techniques of organic synthesis.
C2	Abilities to employ various transformation methods in a multi-step synthesis.
C3	Planning and execution of a complex synthetic sequence based on the literature data.

#### **Relating to skills:**

The person who completed the course:

- PEK\_U01 is able to perform multistep synthesis of an organic compound, select and assemble the appropriate equipment, identify and characterize the products obtained,
- PEK\_U02 can use professional scientific literature and databases to plan the strategy and tactics of the synthesis,
- PEK\_U03 can choose reaction conditions of various transformations, plan the methods of products isolation and purification,

PEK\_U04 - is able to interpret the results, to evaluate the purity of the product by defining basic physicochemical properties, to interpret spectra of organic compounds and to write laboratory notebook in English.

	Form of classes - laboratory	Number of hours
Lab 1	Conducting the laboratory and completion rules. Laboratory notebook. Basic equipment (glass and metal), and laboratory operations. Safety issues: hazardous substances, flammable, etc. Planning the synthesis - the use of the literature and databases.	4
Lab 2	Planning and carrying out the synthesis of two organic compounds (2-4 step sequential processes) using different types of organic	4
Lab 3	reactions: alkylation, acylation, elimination, nucleophilic substitution, electrophilic substitution, oxidation and reduction,	4
Lab 4	cycloaddition. Conversion of alcohols, carbonyl compounds, carboxylic acids and their derivatives, amines, expansion of the	4
Lab 5	carbon scaffold.	4
Lab 6	Purification, identification and characterization of the products.	4
Lab 7	Interpretation of the results, writing the reports.	4
Lab 8	Revision of the laboratory equipment and reports.	2
	Total hours	30

TEACHING TOOLS USED				
N1	planning and execution the experiments			
N2	writing reports (in English)			

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT						
Evaluation	Educational effect	Way of evaluating educational effect				
F – forming (during semester),	number	achievement				
C – concluding (at						
semester end)						
С	PEK_U01 -PEK_U04	Planning and preparation of two organic				
		compounds (2-4 synthetic steps),				
		characterization of the products, writing the				

#### reports.

#### PRIMARY AND SECONDARY LITERATURE

#### PRIMARY LITERATURE:

- [18] A. Mucha, R. Siedlecka, Multistep organic synthesis. practical course, Wrocław, 2010;
- [19] A. I. Vogel, Preparatyka organiczna, WNT, Warszawa, 2006;
- [20] Databases: Beilstein, Chemical Abstracts, Current Contents.

#### **SECONDARY LITERATURE:**

[22] J. Gawroński, K. Gawrońska, K. Kacprzak, M. Kwit, Współczesna synteza organiczna, PWN, Warszawa, 2004

# SUBJECT SUPERVISOR

(NAME AND SURNAME, E-MAIL ADDRESS)

**Renata Siedlecka,** renata.siedlecka@pwr.wroc.pl **Artur Mucha,** artur.mucha@pwr.wroc.pl

## MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

#### **Multistep Organic Synthesis**

#### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

all fields of Faculty of 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***
(skills) PEK_U01	S2Ach4_U06	C1	Lab 2 – Lab 7	N1, N2
PEK_U02	S2Ach4_U06	C3	Lab 1 – Lab 7	N1, N2
PEK_U03	S2Ach4_U06	C2, C3	Lab 1 – Lab 7	N1
PEK_U04	S2Ach4_U06	C1	Lab 2 – Lab 7	N1, N2

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

Zał. nr 4 do ZW 64/2012

# 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 *delete as applicable					

#### **PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES** 1. Non

#### 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		cience and technology? The basic concepts and principles ophy of science and philosophy of technology.	2
Lec 3	The main crit	eria 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 met	thods of inference – induction.	1
Lec 7	The basic met	thods of inference – deduction.	1
Lec 8	The basic me	ethods of inference – abduction.	1
Lec 9,10		ectives and functions of science and technology t of view of classical philosophy of science.	2
Lec 11	from the poin	is and functions of science and technology t of view of the sociology of scientific knowledge.	1
Lec 12, 13		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
Cl 1			hours
Cl 2			
Cl 3			
Cl 4			
	r	Total hours	
		Form of classes – laboratory	Number of hours
Lab1			
Lab2			
Lab3			
Lab4			
Lab5			
		Total hours	
			Number of
		Form of classes – Project	inumber of
Droi1			
Proj1			
Proj2			
Proj3			
Proj4			

		Total hours		
		Form of classes – sem	inar	Number of
Sem1				hours
Sem2				
Sem2				
Sellis				
•••				
		Total hours		
		TEACHING TO	OLS USED	
N1. I	Multimedia present	ation.		
N2. I	Lecture			
N3. I	interactive lecture			
	EVALUATION	NOF SUBJECT EDUCATION	<b>DNAL EFFECTS ACHIEVEMEN</b>	T
Evalı	uation(F – forming	Educationaleffectnumber	Way of evaluating educational eff	ect
	ng semester), P –		achievement	
	luding (at			
seme	ster end)			
F1		PEK_ HUM W07	Passing test, active participatio	n in lectures
		PEK_ HUM W08		
D D1		PEK_HUM K01		
P=F1				
	P	RIMARY AND SECOND	ARY LITERATURE	
PRI	MARY LITERAT	URE:		
[21]	E. Agazzi, Dobro	o, zło i nauka. Etyczny wym	iar działalności naukowo-technic	znej,
	Warszawa 1997;			
[22]	S. Blackburn, Oks	sfordzki słownik filozoficzny	v, Warszawa 2004;	
[23]	A. Chalmers, Czy	m jest to, co zwiemy nauką	Wrocław 1997;	
[24]		Teoria poznania,1994;		
[25]		chmiast, D. Nachmiast, Me	etody badawcze w naukach społe	cznych,
	Poznań 2001;			
		dologia nauk, Kraków 2004		
[27]		udować, mieszkać, myśleć, N	Warszawa 1977;	
		eguny, Warszawa 1985;		
	29] B. Latour, <i>Polityka natury</i> , Warszawa 2009;			
	<ul> <li>K.R. Popper, Wiedza obiektywna, Warszawa 1992;</li> <li>J. Woleński, Epistemologia, Warszawa 2005.</li> </ul>			
[31]	J. WOIENSKI, Epis	<i>iemologia</i> , warszawa 2005		
SFC	ONDARY LITER	ATURF.		
			nontalism Toopationen Dourse	ntaoja
[23]	[1] D. Sobczynska Poznań 1994,	, r. Zeiuier, ivowy eksperyn	nentalizm. Teoretycyzm. Repreze	niacja,

[24] P. Zeidler, Spór o status poznawczy teorii, Poznań 1992.

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

Marek Sikora m.sikora@pwr.wroc.pl

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

# SCIENCES

501	ENCES			
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

# **SUBJECT CARD**

Name in Polish	Fizyczna chemia organiczna
Name in English	Physical organic chemistry
Main field of study (if applicable)	
Specialization (if applicable)	Medicinal chemistry
Level and form of studies:	1st/ 2nd* level, full-time
Kind of subject	obligatory
Subject code	CHC024013
Group of courses	NO
*delete as applicable	

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of					
organized classes in	15				
University (ZZU)					
Number of hours of total					
student workload (CNPS)					
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-	1				
student contact (BK) classes					

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

21. Knowledge of organic chemistry, theoretical and practical

	SUBJECT OBJECTIVES		
C1	Learning the type of molecular interactions		
C2	Learning the basic kinetic and thermodynamic phenomena		
C3	Learning acid base interaction		
C4	Learnng basics of reaction mechanism in organic chemistry		
C4	Learning the symmetry relation within molecule		

**Relating to knowledge:** PEK\_W01 – He understands the basic thermodynamics. PEK\_W02 – He is able to write and predict reaction mechanism PEK\_W03 – He is able to define the symetry of the molecule PEK\_W04 – He is able to define the type of intra and inter molecular interactions

	PROGRAMME CONTENT				
	Form of classes - lecture	Number of hours			
Lec 1-2	Bonds in organic chemistry	2			
Lec 3-4	Intermolecular forces	2			
Lec 5-6	Reactive intermediates	2			
Lec 7-8	Reaction mechanism, nucleophilic and electrophilic mechanism	2			
Lec 9-10	Reaction mechanism, radical mechanism	2			
Lec 11-12	Symetry of molecules	2			
13-14	Acid base equilibria	2			
Lec 15	Evaluation test	1			
	Total hours	15			

	TEACHING TOOLS USED
N1	Lecture with multimedial presentation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT					
Evaluation	Educational effect	Way of evaluating educational effect			
F – forming (during semester), C – concluding (at semester end)	number	achievement			
P1	W1-W15	test			

#### **PRIMARY LITERATURE:**

- [32] Bruckner Bernard Organic mechanisms, reactions, stereochemistry and synthesis
- [33] Jones Richard, Physical and mechanistic organic chemistry
- [34] Carter Robert, Molecular symmetry and group theory

#### **SECONDARY LITERATURE:**

- [25] Ilich, Predrag Peter, Selected problems in physical chemistry
- [26] Deslongchamps, Stereoelectronis effects in organic chemistry
- [27] Jaffe, Hans Symmetry in chemistry

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

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## MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Physical organic chemistry

#### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

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 content***	Teaching tool number***
(knowledge) PEK_W01	S2Ach4-W07	C1	Le1-Le4	N1
(knowledge) PEK_W02	S2Ach4-W07	C2	Le7-Le8	N1
(knowledge) PEK_W03	S2Ach4-W07	C4	Le11-Le12	N1
(knowledge) PEK_W04	S2Ach4-W07	C1 ,C3	Le1-Le4	N1

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

# **SUBJECT CARD**

Name in Polish <b>Podstaw</b>	y Chemii Fizjologicznej
Name in English <b>Princip</b>	les of Physiological Chemistry
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	Medicinal Chemistry
Level and form of studies:	2nd* level, full-time
Kind of subject	optional
Subject code	CHC020038
Group of courses	YES / 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	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					
including number of ECTS points for practical (P) classes					
including number of ECTS points for direct teacher-					
student contact (BK) classes *delete as applicable					

\*delete as applicable

#### PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER **COMPETENCES**

1. The student knows biology on the high school level.

	SUBJECT OBJECTIVES				
C1	Knowledge of chemical compounds that build a living organism.				
<u>C2</u>	Understanding the basic laws governing the metabolism of living organisms				
C2	Understanding the basic laws governing the metabolism of living organisms.				
C3	Understanding the basic laws governing selected biochemical processes				

**Relating to knowledge:** PEK\_W01 is familiar with the basic principles of biochemistry PEK\_W02 knows structures and functions of main types of macromolecules PEK\_W03 has a basic knowledge of energy conversions occurring in living organisms PEK\_W04 is able to characterize the biochemical process

	PROGRAMME CONTENT				
	Form of classes - lecture				
Lec 1	From amino acids and peptides to proteins and their function.	2			
Lec 2	Structure and functioning of DNA and RNA.	2			
Lec 3	Structure and functioning of fatty acids.	2			
Lec 4	Carbohydrates and their function.	2			
Lec 5	Small molecules in signal transduction.	2			
Lec6	Structure and functioning of membrane.	2			
Lec 7	Review of cytoplasmic organelles.	2			
Lec 8	Meiosis and Mitosis	2			
Lec 9	Cell death processes.	2			
Lec 10	Processes of intra and extracellular signal transduction.	2			
Lec 11	Processes of intra and extracellular metabolism regulation.	2			
Lec 12	Additional comments.	2			
Lec 13	Seminar.	2			
Lec 14	Seminar.	2			
Lec 15	Seminar.	2			
	Total hours	30			

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT			
<b>Evaluation</b> F – forming (during semester),	Educational effect number	Way of evaluating educational effect achievement	
C – concluding (at semester end)			
F1	PEK_W01 do PEK_W04	Participation in the lectures	
C – grade for quality of presented seminar			

#### **PRIMARY LITERATURE:**

[35] Jeremy M. Berg, Lubert Stryer, John L. Tymoczko, Biochemistry, Sixth Edition[36] John C. McMurry. Organic Chemistry

#### **SECONDARY LITERATURE:**

[28] Pharmaceutical Bioassays – Methods and Applications, Shiqi Peng, Ming Zhao, Wiley 2009

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

Dr hab. Marcin Drąg, prof. Pwr, <u>marcin.drag@pwr.wroc.pl</u>

## MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Principles of Physiological Chemistry

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

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 content***	Teaching tool number***
(knowledge) PEK_W01	K1Ach_W15	C1	Lec3, Lec 5, Lec 7, Lec 6	N1
PEK_W02	K1Ach_W15	C1	Lec 1, Lec 2, Lec 4,	N1
PEK_W03	K1Ach_W15	C2	Lec 10, Lec 11	N1
PEK_W04	K1Ach_W15	C3	Lec 8, Lec 9, Lec 12	N1

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

# SUBJECT CARD

Name in Polish	Polimery w medycynie	
Name in English	Polymers in medicine	
Main field of study (if applicable)	Chemistry	
Specialization (if applicable)	Medicinal chemistry	
Level and form of studies:	1st/ 2nd* level, full-time	
Kind of subject	obligatory	
Subject code	CHC024055	
Group of courses	NO	

\*delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of					
organized classes in	15				
University (ZZU)					
Number of hours of total	60				
student workload (CNPS)	00				
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-	0.5				
student contact (BK) classes					

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

22. Completed course of organic chemistry

23.

 $\frac{C1}{C2}$ 

# SUBJECT OBJECTIVES To show how polymers can be used in medicine To describe specificity of polymers

C3 To allow designing of new medical appliances from polymers

**Relating to knowledge:** PEK\_W01 – to have a knowledge on preparation and properties of polymers PEK\_W02 – to know the place of polymers in construction of drug delivery systems PEK\_W03 – to know how to use polymers as artificial implants, PEK\_W04 – is able to predict the use of particular polymer

	PROGRAMME CONTENT	
	Form of classes - lecture	Number of hours
Lec 1	History of polymers, definitions, properties of polymers	2
Lec 2	Molecular weights, polydispersity, determination of molecular weight	2
Lec 3	Polyaddtion and polycondensation, properties of polymers	2
Lec 4	Soluution of polymers, Thermodynamics, phase separation	2
Lec 5	Polymers in condensed phase, blends, phase transitions, characteristic temperatures	2
Lec 6	Mechanical properties of polymers	2
Lec 7	Surfaces, modification and evaluation	2
Lec 8	Transport phenomena in polymers, Fickian an abnormal diffusion	2
Lec 9	Artificial kidney – history and perspectives	2
Lec 10	Artificial organs: liver, lung and skin	2
Lec 11	Polymer scaffolds, preparation and the use in tissue emgineering	2
Lec 12	Polymer auxalities in medicine and pharmacy	2
Lec 13	Polymers in drug production, separation, membrane systems, polymers in water treatment	2
Lec 14	Discussion forum on the use of polymes to implants	2
Lec 15	Discussion forum on the use of polymers in designing of new drugs	2
	Total hours	30

	TEACHING TOOLS USED
N1	Lecture
N2	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	
F1	Lecture	Activity	

6 suggestions on the use of polymers 5.5 (A) 5 suggestions on the use of polymers 5 (B) 4 suggestions on the use of polymers 4.5 (C)
3 suggestions on the use of polymers 4 (D 2 suggestions on the use of polymers 3,5 (E 1 suggestion on the use of polymers 3 (E

C

#### PRIMARY AND SECONDARY LITERATURE

#### PRIMARY LITERATURE:

[37] M.Bryjak, I.Gancarz, Polymers in medicine, wyd PWr 2010

#### **SECONDARY LITERATURE:**

- [29] L.H.Sperling, Introduction to physical polymer science
- [30] F.Billmayer, Textbook of polymer science,

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

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# MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Polymers in medicine

#### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

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	S2Ach4_W05	C2	W1-W8	N1, N2
PEK_W02	S2Ach4_W05	C1, C3	W9-W13, W15	N1, N2
PEK_W03	S2Ach4_W05	C1, C3	W9-W13, W14	N1, N2
PEK_W04	S2Ach4_W05	C1, C3	W14, W15	N1, N2

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

# **SUBJECT CARD**

Name in Polish Podstawy	y Chemii Fizjologicznej	
Name in English <b>Principles of Physiological Chemistry</b>		
Main field of study (if applicable)	Chemistry	
Specialization (if applicable)	Medicinal Chemistry	
Level and form of studies:	2nd* level, full-time	
Kind of subject	optional	
Subject code	CHC020038	
Group of courses	YES / NO*	
*delete as applicable		

Lecture	Classes	Laboratory	Project	Seminar
30				
60				
crediting with grade*	Examination / crediting with grade*	Examination / crediting with grade*	Examination / crediting with grade*	Examination / crediting with grade*
	30 60 crediting	30 60 crediting Examination	30     Examination       60     Fraction       crediting     Examination       with grade*     / crediting	30     Examination       60     Examination       crediting     Examination       with grade*     / crediting

\*delete as applicable

#### PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER **COMPETENCES**

1. The student knows biology on the high school level.

	SUBJECT OBJECTIVES		
C1	Knowledge of chemical compounds that build a living organism.		
C2	Understanding the basic laws governing the metabolism of living organisms.		
C3	Understanding the basic laws governing selected biochemical processes		

**Relating to knowledge:** PEK\_W01 is familiar with the basic principles of biochemistry PEK\_W02 knows structures and functions of main types of macromolecules PEK\_W03 has a basic knowledge of energy conversions occurring in living organisms PEK\_W04 is able to characterize the biochemical process

PROGRAMME CONTENT				
	Number of hours			
Lec 1	From amino acids and peptides to proteins and their function.	2		
Lec 2	Structure and functioning of DNA and RNA.	2		
Lec 3	Structure and functioning of fatty acids.	2		
Lec 4	Carbohydrates and their function.	2		
Lec 5	Small molecules in signal transduction.	2		
Lec6	Structure and functioning of membrane.	2		
Lec 7	Review of cytoplasmic organelles.	2		
Lec 8	Meiosis and Mitosis	2		
Lec 9	Cell death processes.	2		
Lec 10	Processes of intra and extracellular signal transduction.	2		
Lec 11	Processes of intra and extracellular metabolism regulation.	2		
Lec 12	Additional comments.	2		
Lec 13	Seminar.	2		
Lec 14	Seminar.	2		
Lec 15	Seminar.	2		
	Total hours	30		

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT					
<b>Evaluation</b> F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement			
F1	PEK_W01 do PEK_W04	Participation in the lectures			
C – grade for quality of presented seminar					

#### **PRIMARY LITERATURE:**

[38] Jeremy M. Berg, Lubert Stryer, John L. Tymoczko, Biochemistry, Sixth Edition[39] John C. McMurry. Organic Chemistry

#### **SECONDARY LITERATURE:**

[31] Pharmaceutical Bioassays – Methods and Applications, Shiqi Peng, Ming Zhao, Wiley 2009

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

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#### MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

Principles of Physiological Chemistry

AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

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 content***	Teaching tool number***
(knowledge) PEK_W01	K1Ach_W15	C1	Lec3, Lec 5, Lec 7, Lec 6	N1
PEK_W02	K1Ach_W15	C1	Lec 1, Lec 2, Lec 4,	N1
PEK_W03	K1Ach_W15	C2	Lec 10, Lec 11	N1
PEK_W04	K1Ach_W15	C3	Lec 8, Lec 9, Lec 12	N1

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

# **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)	<b>Bioinformatics, Medicinal Chemistry</b>
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	30				
University (ZZU)					
Number of hours of total	90				
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-	1				
student contact (BK) classes					

\*delete as applicable

#### PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER **COMPETENCES**

24. Knowledge of basic organic chemistry25. 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			

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

	techniques.	
Lec12	<b>Selective complexation of metalloenzymes.</b> History of the discovery of captopril. Convertase as a target for anti-hypertensive drugs. Choice of ligand.	2
Lec13	<b>Drug targeting and delivery.</b> 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	<b>Gene therapy.</b> 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 LITERATURE:**

- 1. K. M. Merz, Drug Design, structure and Ligand-Based Approaches, Cambridge University Press, 2010
- 2. Medicinal Chemistry and Drug Design, e d. D. Dnkici, Intech (open access), 2012

#### **SECONDARY LITERATURE:**

- 1. Design of Drugs: Basic Principles and applications, ed. J. H. Poupaert, Marcel Dekker, 2002
- 2. The Organic Chemistry of Drug Design and Drug Action, Academic Press, 2004
- 3. Virtual Screening. ed. M. O. Taha, Intech (open access), 2012
- 4. Drug Development A Case study Based Insight intor Modern Startegies, Intech (open access), 2011

## SUBJECT SUPERVISOR

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Prof.dr hab. inż. Paweł Kafarski, pawel.kafarski@pwr.wroc.pl

# 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

### **SUBJECT CARD**

Informacja naukowa i techniczna w biotechnologii		
Retrieval of scientific and technical		
information		
Biotechnology, Chemistry		
<b>Bioinformatics, Medicinal chemistry</b>		
2 <sup>nd</sup> level, full-time		
obligatory		
INC024008		
NO		

delete as applicable

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of					
organized classes in			15		
University (ZZU)					
Number of hours of total			30		
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			1		
points for practical (P) classes			1		
including number of ECTS					
points for direct teacher-			0.5		
student contact (BK) classes					

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

26. Basic computer science skills

Communication in English language 27.

#### 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	N2 Solving problems		
N3	Use of compter software to solve problems		

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT					
Evaluation	Educational effect	Way of evaluating educational effect			
C – concluding (at	number	achievement			
semester end)					
С	PEK_U02	Final report maximum 100 score points			
С	PEK_U03	grade 3.0 for 50-60 score points			
С	PEK_U04	grade 3.5 for 61-70 score points			
С	PEK_U05	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			

### **PRIMARY LITERATURE:**

[1] D. Ridley, Finding scientific information – information retrieval, Wiley, 2002

# SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS) W. Andrzej Sokalski, sokalski@pwr.wroc.pl

### 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

### **SUBJECT CARD**

Name in Polish	Wybrane reakcje w chemii organicznej
Name in English	Selected reactions in organic chemistry
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	Medicinal Chemistry
Level and form of studies:	2nd level, full-time
Kind of subject	optional
Subject code	CHC0240044
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	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	0.5				

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1 Passed lecture on "Principles of Organic Chemistry"

2 Knowledge of the basic mechanisms of organic reactions

3 Knowledge of English

#### SUBJECT OBJECTIVES

C1	Presentation of the basic classes of organic compounds including the question of isomerism, stereochemistry, and the most important characteristic of the reaction of
	functional groups.
C2	Presentation of the selected mechanisms of organic name reactions, and a number of
	other reactions.
C3	Discussion of the mechanisms of organic reactions such as addition, elimination,
	radical substitution, electrophilic and nucleophilic substitution
C4	Discussion of pericyclic reaction.
C5	Discussion of the reactions of organometallic compounds.
C6	Discussion of the planning principles established synthesis of the target molecule

### SUBJECT EDUCATIONAL EFFECTS

### **Relating to knowledge:**

The person who passed the course

- PEK\_W01 knows the basic classes of organic compounds including the question of isomerism, stereochemistry, and the most important characteristic of the reaction of functional groups.
- PEK\_W02 know the mechanisms of organic reactions such as addition, elimination, substitution radical, electrophilic and nucleophilic and selected name reactions
- PEK\_W03 known reactivity of organometallic compounds and phosphorous- and sulfur organic compounds and examples of their use in the synthesis
- PEK\_W04 known selective reduction methods and selective oxidation method used in organic chemistry

PEK\_W05 - understand the purpose and know how to protect the functional groups

PEK\_W06 – know what to do when planning a synthesis of the target molecule for moderately complex structure

	PROGRAMME CONTENT		
	Form of classes - lecture	Number of hours	
Lec 1	Electronic structure of organic compounds.	2	
Lec 2	Molecular architecture – elements of stereochemistry.	2	
Lec 3	Reaction equilibrium and rate.	2	
Lec 4	Intermediates, transition state.	2	
Lec 5	Reactions of aromatic compounds.	2	
Lec 6	Reactions of carbonyl compounds.	2	
Lec 7	Reactions of some organometallic compounds (Li, Mg, Zn,).	2	
Lec 8	Reactions of organophosphorous and sulfur compounds.	3	
Lec 9	Pericyclic reactions.	2	
Lec 10	Selective methods for reductions of organic compounds.	2	
Lec 11	Selective methods for oxidations of organic compounds.	2	
Lec 12	Ideas of organic synthesis.	2	
Lec 13	Selective transformations and protections of functional groups.	3	
Lec 14	Targeted synthesis.	2	
	Total hours	30	

	TEACHING TOOLS USED
N1	lecture and multimedia presentation

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT					
<b>Evaluation</b> F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement			
credit		on the basis of student's attendance			

### **PRIMARY LITERATURE:**

[40] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford, 2000;

[41] J. McMurry, Chemia organiczna, tom 1 – 5, PWN, Warszawa, 2005;

[42] Michael B. Smith, Jerry March, March's Advanced Organic Chemistry, Wiley, 2000.

[43] J. Skarzewski, Wprowadzenie do syntezy organicznej, PWN, Warszawa, 1999.

### **SECONDARY LITERATURE:**

[32] L. G. Wade, Organic Chemistry, Prentice Hall, Upper Saddle River, NJ, 2006.

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

Professor. Dr. hab. Jacek Skarżewski, jacek.skarzewski @ pwr.wroc.pl

### MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

### Selected reactions in organic chemistry AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

### Chemistry AND SPECIALIZATION 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 content***	Teaching tool number***
(knowledge)	optional course	C1	Lec 1- Lec 3,	N1

PEK_W01		Lec 13	
PEK_W02	C2-C4	Lec 4- Lec 9	N1
PEK_W03	C5	Lec 7, Lec 8	N1
PEK_W04	C2-C5	Lec 10, Lec 11	N1
PEK_W05	C2-C5	Lec 13	N1
PEK_W06	C6	Lec 12, Lec 14	N1

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

### SUBJECT CARD

Name in Polish	Spektroskopia	
Name in English	Spectroscopy	
Main field of study (if applicable)	Chemistry	
Specialization (if applicable)		
Level and form of studies:	2nd level, full-time	
Kind of subject	obligatory	
Subject code	CHC024031	
Group of courses	NO	
Group of courses		

	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	Examination		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			1		

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

- 28. Knowledge of general chemistry
- 29. Basic knowledge of physical chemistry
- 30. Ability of using the mathematical analysis
- 4. Basic physicochemical calculations
- 5. Basic knowledge of the atomic and molecular spectroscopy.

	SUBJECT OBJECTIVES		
C1	Acquisition of knowledge on selected experimental methods of measuring rotational		
	and vibrational spectra, and on measuring equipment		
C2	Acquisition of knowledge of measurement techniques of photoelectron spectra		
	(PES), Auger electrons and the X-ray fluorescence.		
C3	Acquisition of knowledge on electron spectroscopy of polyatomic molecules		
	including application of the group theory in chemistry.		
C4	Acquisition of knowledge on methods of detection of absorption and luminescence		
	spectra of polyatomic molecules, in particular of spectra with highly resolved		

	vibronic structure
C5	Acquisition of knowledge about of interpretation of two-dimensional spectra of the
	nuclear magnetic resonance (COSY)
C6	Getting acquainted with selected applications of the atomic and molecular
	spectroscopy

SUBJECT EDUCATIONAL EFFECTS
Relating to knowledge:
Having completed the course, the student:
PEK_W01 – has a basic knowledge on selected experimental methods of measuring
rotational and vibrational spectra, and on measuring equipment
PEK_W02 – knows principles of the spectroscopy of photoelectrons (PES), Auger electrons
and the X-ray fluorescence
PEK_W03 – has a basic knowledge of molecular spectrometry with particular reference to
electronic-vibrational spectroscopy of two- and polyatomic molecules and to
techniques allowing to acquire two-dimensional spectra of high resolution
PEK_W04 – has a knowledge on classification of molecules taking into account their
symmetry and is able to apply the group theory in chemistry.
PEK_W05 – can interprete two-dimensional spectra of the nuclear magnetic resonance
(COSY)
Relating to skills:
Having completed the course, the student:
PEK_U01 – is able to prepare samples, and to measure and interpret vibrational spectra,
PEK_U02 – can interpret NMR spectra and, based on the interpretation, can determine
structure of an organic molecule,
PEK_U03 – is able to use UV-VIS absorption spectra to determine kinetic parameters of
photochemical reactions,
PEK_U04 – is able to use the emission spectroscopy to determine fundamental parameters
of the atomic structure
PEK_U05 – is able to interpret the fine rotational structure of vibronic bands in
spectra of diatomic molecules
Relating to social competences:
Having completed the course, the student:
PEK_K01– acquired knowledge of the rotational, vibrational and electron spectroscopy to
the degree enabling him/her a creative use of scientific literature, and developing
and presentation of related issues

	PROGRAMME CONTENT			
	Form of classes - lecture	Number of hours		
Lec 1	Rotational and vibrational spectroscopy, experimental methods: light sources, Fourier techniques, detectors	4		
Lec 2	Spectroscopy of photoelectrons (PES), Auger electrons and the X-ray fluorescence.	2		
Lec 3	Application of the group theory in chemistry.	2		
Lec 4	Two-dimensional electron spectra of polyatomic molecules and	3		

	highly resolved vibronic luminescence spectra with the application: spectroscopy in supersonic nozzles, spectroscopy of single molecules, laser selection of sites.	
Lec 5	Nuclear magnetic resonance (NMR) and multidimensional spectra (COSY)	4
	Total hours	15

	Form of classes - laboratory	Number of hours
Lab 1	Schedule of classes. Principles of the credit. Principles of the safe work in the chemical laboratory.	2
Lab 2	Infrared spectroscopy - preparation of samples, measurements of spectra and their interpretation.	4
Lab 3	Raman spectroscopy - preparation of samples, comparing IR and Raman spectra	4
Lab 4	Introduction to one and of two-dimensional NMR techniques - recording of spectra.	4
Lab 5	Analysis and interpretation of 1-D and 2-D NMR spectra	4
Lab 6	Photochromism - determination of the photochromic reaction rate constant.	4
Lab 7	Determination of atomic constants from emission spectra.	4
Lab 8	Analysis of rotational structure of $N^{2+}$ spectra - determination of rotational constants and distances between nitrogen atoms.	4
	Total hours	30

	TEACHING TOOLS USED		
N1	Problem lectures - multimedia presentations		
N2	Laboratory work - instructions to all exercises available online		
N3	Independent student's work - writing reports on laboratory exercises		
N4	Consultation		
N5	Independent work - preparation for the final examination		

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		
C1	PEK_W01 PEK_W02 PEK_W03 PEK_W04 PEK_W05	Grade from a written exam		
F1	PEK_U01 PEK_U05	Report on exercises		

### **PRIMARY LITERATURE:**

- [44] K. Pigoń, Z. Ruziewicz, Chemia fizyczna t 2 Fizykochemia molekularna, Wyd. PWN, Warszawa 2007
- [45] P.W. Atkins, Chemia fizyczna, PWN 2001
- [46] R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spektroskopowe metody identyfikacji związków organicznych PWN, Wraszawa 2007.
- [47] D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Podstawy chemii analitycznej 2, PWN, Warszawa 2007.
- [48] Z. Kęcki, Podstawy spektroskopii molekularnej, Wyd. PWN, Warszawa 1992.

### **SECONDARY LITERATURE:**

- [33] A. Cygański, Metody spektroskopowe w chemii analitycznej. WNT Warszawa, 2009
- [2] J. Demichowicz-Pigoniowa, Chemia fizyczna t 3, Obliczenia fizykochemiczne, PWN, Warszawa 2010
- [3] W. Zieliński, A. Rajca, Metody spektroskopowe i ich zastosowanie do identyfikacji związków organicznych, WNT, Warszawa 2000.
- [4] J. Najbar, A. Turek, Fotochemia i spektroskopia optyczna, PWN, Warszawa 2009.
- [5] P. Suppan, Chemia i światło, PWN, Warszawa 1997.

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

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### MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

### Spectroscopy

### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

### 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	K2Ach_W03: X2A_W01, X2A_W03 X2A_W05, X2A_W06	C1	Lec1	N1, N5
PEK_W02	K2Ach_W03; X2A_W00 K2Ach_W03: X2A_W01, X2A_W03 X2A_W05, X2A_W06	C2	Lec2	N1, N5
PEK_W03	K2Ach_W03: X2A_W01, X2A_W03 X2A W05' X2A W06	C3, C4	Lec3	N1, N5
PEK_W04	K2Ach_W03: X2A_W01, X2A_W03 X2A_W05, X2A_W06	C3,C4	Lec3,Lec4	N1, N5
PEK_W05	K2Ach_W03: X2A_W01, X2A_W03 X2A_W05, X2A_W06	C5	Lec5	N1, N5
(skills) PEK_U01	K2Ach_U03: X2A_U01, X2A_U02 InżA U01	C6	Lab2, Lab3	N2, N3, N4
PEK_U02	K2Ach_U03: X2A_U01, X2A_U02 InżA U01	C6	Lab4, Lab5	N2, N3, N4
PEK_U03	K2Ach_U03: X2A_U01, X2A_U02 InżA U01	C6	Lab6	N2, N3, N4
PEK_U04	K2Ach_U03: X2A_U01, X2A_U02 InżA U01	C6	Lab7	N2, N3, N4
PEK_U05	K2Ach_U03: X2A_U01, X2A_U02 InżA_U01	C6	Lab8	N2, N3, N4
(competences) PEK_K01	K2Ach_W03: X2A_W01, X2A_W03 X2A_W05, X2A_W06 K2Ach_U03: X2A_U01, X2A_U02 InżA_U01	C1C6	Lec1-Lec5 Lab2-Lab8	N1-N5

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

\*\*\* - from table above

### **SUBJECT CARD**

Name in Polish	Syntetyczne Leki Organiczne
Name in English	Synthetic Organic Drugs
Main field of study (if applicable)	Chemistry
Specialization (if applicable)	Medicinal Chemistry
Level and form of studies:	2nd level, full-time
Kind of subject	obligatory
Subject code	CHC024017
Group of courses	YES
*delete as applicable	

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of					
organized classes in	30		60		
University (ZZU)					
Number of hours of total					
student workload (CNPS)					
Form of crediting	Examination		Crediting with grade		
For group of courses mark					
(X) final course					
Number of ECTS points	3		4		
including number of ECTS points for practical (P) classes			4		
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

- 31. Principles of organic chemistry, theoretical and practical.
- 32. Basic knowledge of biochemistry.
- 33. Knowledge in the field of basis of analytical chemistry is recommended.

	SUBJECT OBJECTIVES		
C1	Introduction to the type of drug targets.		
C2	Basic important places and molecules as potential drug targets.		
C3	The strategy of action of particular classes of drugs.		
C4	Acquaintance with the different concepts in the field of analysis of the biological		
C4	active components of drugs, depending of the drug formulation.		
C5	Gaining of the knowledge on the strategies of isolation of the biologically active		
	compounds from a drug form, in order to do qualitative and quantitative analyzes of		
	the separated substances.		

### SUBJECT EDUCATIONAL EFFECTS

### **Relating to knowledge:**

Student, who has completed the course:

PEK\_W01 - has knowledge on the main drug targets,

PEK\_W01 – has knowledge on the strategy of action of basic classes of drugs,

PEK\_W02 – can define the possible mechanisms of action of main drug classes.

### **Relating to skills:**

Student, who has completed the course:

- PEK\_U01 has skills of using different separation techniques to isolate biologically active compounds from the different types of drug formulations,
- PEK\_U02 has skills to do qualitative analysis of the biologically active components of drugs using the characteristic reactions,
- PEK\_U03 has skills to do quantitative analysis of the biologically active components of drugs using different analytical techniques,
- PEK\_U04 has skills to do synthesis of a biologically active compound and to be able to compare it to the same isolated from a drug by qualitative analysis,
- PEK\_U05 has skills to prepare a laboratory report according to Good Laboratory Practice rules,
- PEK\_U06 has skills to characterize a biologically active compound of a drug using spectroscopic techniques: NMR, FT-IR and MS.

	PROGRAMME CONTENT				
Form of classes - lecture					
Lec 1	Introduction to the type of drugs targets.	2			
Lec 2	Basic important organelles in the living system, potential drug targets	2			
Lec 3	Basic important biological molecules and macromolecules, potential drugs targets.	2			
Lec 4	Review on the molecular interactions important in biology.	2			
Lec 5	Drugs interacting with lipids, mechanism of interaction.	2			
Lec 6	Drugs interacting with lipids, mechanism of interaction.	2			
Lec 7	Drugs interacting with proteins, mechanism of interaction.	2			
Lec 8	Drugs interacting with DNA and RNA, mechanism of interaction.	2			
Lec 9	Strategy of action of anti-fungi drugs.	2			
Lec 10	Strategy of action of antiviral drugs.	2			
Lec 11	Strategy of action of antibacterial drugs.	2			
Lec 12	Strategy of action of anticancer drugs.	2			
Lec 13	Drug metabolism and toxicity.	2			
Lec 14	Elements of pharmacokinetics and pharmacodynamics.	2			
Lec 15	The selected case studies part 2.	2			
	Total hours	30			

	Number of hours	
Lab 1	Safety rules in the laboratory of organic chemistry, good laboratory	4

	preserves and the miles of the reports preparation. Introduction to the	
	practice and the rules of the reports preparation. Introduction to the	
	separation and identification techniques in the organic chemistry	
	laboratory. NMR, FT-IR and MS spectra analyzes rules.	
Lab 2	Paracetamol – quantitative and qualitative analyzes of one biologically	4
	active ingredient drug.	-
Lab 3	NO-SPA – quantitative and qualitative analyzes of drotaverine	4
	hydrochloride from a tablet.	I
Lab 4	Pyralginum – isolation, quantitative and qualitative analyzes of	4
	metamizole sodium from a tablet.	4
Lab 5	Ascodan – two compounds drug – isolation and separation of	4
	acetylsalicylic acid and codeine phosphate from a tablet.	4
Lab 6	Ascodan – two compounds drug - quantitative and qualitative analyzes of	Α
	acetylsalicylic acid and codeine phosphate.	4
Lab 7	Etopiryna – three compounds drug in a tablet form –separation techniques	4
	in the isolation of acetylsalicylic acid, ethenzamide and caffeine.	4
Lab 8	Etopiryna – three compounds drug in a tablet form – qualitative and	
Luc c	quantitative analyzes of acetylsalicylic acid, ethenzamide and caffeine.	4
Lab 9	Cardiamidum – a drug in a form of drops (liquid formulation) -	
	quantitative and qualitative analyzes of cardiamide and lactic acid.	4
Lab 10	Unguentum undecylenicum – isolation of the biologically active	
Luo 10	components from the ointment form of a drug.	4
Lab 11	Unguentum undecylenicum – qualitative and quantitative analyzes of	
	undecylenic acid and its zinc salt form.	4
Lab 12	Ibuprophen – a suspension form of a drug – isolation techniques,	
La0 12	qualitative and quantitative analyzes.	4
Lab 13	Guaiaphenezin – Wiliamson ether synthesis from guaiacol – a component	
La0 15		4
T 1 1 4	of suspensions and tablets. Isolation of guaiaphenezin from a tablet.	
Lab 14	The comparison of qualitative and quantitative analyzes results of	4
T 1 4 -	guaiaphenezin isolated from tablet mass with this synthesized.	
Lab 15	Analyzes of NMR, FT-IR and MS spectra of the isolated biologically	4
	active components of drugs during labs meetings. Repeating of the not	4
	successful realized experiments.	
	Total hours	60

TEACHING TOOLS USED		
N1	Lecture with multimedial presentation.	
N2	Experiment realizing.	
N3	Report preparation.	

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT					
<b>Evaluation</b> F – forming (during semester), P – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement			
P1	PEK_W01-W02	The exam			
F1(laboratory)	PEK_U01 – U05	Completed 9 reports, containing results,			

		calculations and conclusions, prepared according to good laboratory practice rules	
F2 (laboratory)	PEK_U06	NMR, FT-IR and MS spectra analyzes of every of the biologically active components isolated by a student during laboratory meetings (13 completed analyzes).	
P2 (laboratory)– $(F1 \pm F2)/2$			

### P2 (laboratory) = (F1 + F2) / 2

### PRIMARY AND SECONDARY LITERATURE

### **PRIMARY LITERATURE:**

- [49] Partick, Graham, An introduction to medicinal chemistry
- [50] Farrell Susan, Principles of Pharmacology
- [51] Moynihan, Humphrey A. The physicochemical basic of pharmaceuticals.
- [52] R Gancarz, Synthetic organic drug. Script for Medicinal Chemistry Politechnika Wrocławska, 2011.
- [53] I Pawlaczyk, R Gancarz, Synthetic organic drugs. Labotaroty. Drugs analysis. Script for Medicinal Chemistry Politechnika Wrocławska, 2011.
- [54] AC Moffat, MD Osselton, B Widdop, Clarke's analysis of drugs and poisons. Pharmaceutical Press, 2005.

### **SECONDARY LITERATURE:**

- [34] Testa Berbnard, The biochemistry of drug metabolism
- [35] Donald J. Abraham, Burgers Medicinal Chemistry and Drug Discovery vol 1-6
- [36] Collen Smith, and co. Marks' Basic Medical Biochemistry A Clinical Approach
- [37] Farmakopea Polska V, Urząd Rejestracji Leków, Wyrobów Medycznych I Produktów Biobójczych, Warszawa, 1990.
- [38] M Gorczycowa, A Zejc, Ćwiczenia z chemii leków, praca zbiorowa. Collegium Medicum UJ, Kraków, 1996.
- [39] R Kasprzykowska, AS Kołodziejczyk, Chemiczna analiza środków leczniczych (leki proste). Skrypt z chemii leków. Uniwersytet Gdański, Gdańsk, 2010.

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

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### MATRIX OF CORRELATION BETWEEN EDUCATIONAL EFFECTS FOR SUBJECT

### Synthetic Organic Drugs

### AND EDUCATIONAL EFFECTS FOR MAIN FIELD OF STUDY

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 content***	Teaching tool number***
PEK_W01	S2Ach4-W01	C1,C2	Lec1-Lec8	N1
PEK_W02	S2Ach4-W01	C1,C2	Lec9-Lec12	N1
PEK_W03	S2Ach4-W01	C1,C2,C3	Lec13-Lec15	N1
PEK_U01	S2Ach4_U01	C4	Lab1, Lab4, Lab5, Lab7, Lab9, Lab10, Lab12, Lab13	N1
PEK_U02	S2Ach4_U01	C5	Lab1, Lab2, Lab3, Lab4, Lab6, Lab8, Lab9, Lab11, Lab12, Lab14, Lab15	N2, N3
PEK_U03	S2Ach4_U01	C5	Lab2, Lab3, Lab4, Lab6, Lab8, Lab9, Lab11, Lab12, Lab14	N2, N3
PEK_U04	S2Ach4_U01	C4, C5	Lab13, Lab14	N2, N3
PEK_U05	S2Ach4_U01	C4, C5	Lab1 – Lab15	N2, N3
PEK_U06	S2Ach4_U01	C4	Lab1, Lab2, Lab3, Lab4, Lab6, Lab8, Lab9, Lab11, Lab12, Lab14, Lab15	N3

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

\*\*\* - from table above

### **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- student contact (BK) classes	1	0.5	1		

\*delete as applicable

# PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

34. General Chemistry, Physics I and II

35. Algebra, Mathematical Analysis

36. 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	<b>Classical and quantum mechanics</b> . 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	<b>The foundations of quantum mechanics</b> . Postulates of quantum mechanics. The definition of wavefunction and its probabilistic interpretation. The definition of operators representing observables.	2	
Lec 3	<b>The foundations of quantum mechanics II</b> . 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	<b>Hydrogen atom</b> . 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.	2	

	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.	
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	<b>Molecule.</b> 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	<b>Chemical bond.</b> Electrostatic and covalent character of chemical bonds. Type of bonds. Orbitals $\sigma$ and $\pi$ . Bonding, antybonding, and nonbonding orbitals – energies and geometrical representation. The electronic structure of diatomic molecules. The bond order.	2
Lec 10	<b>Localized orbitals.</b> 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	<b>Molecular spectroscopy I.</b> The rotation and vibration separation. Rotational spectra of diatomic molecules and elements of microwave spectroscopy. The selection rules.	2
Lec 12	<b>Molecular spectroscopy II.</b> Vibarational spectra of diatomic and many-atoms molecules. IR and Raman spectra. The selection rules.	2
Lec 13	<b>Molecular properties based on energy.</b> 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.	
Lec 15	<b>Molecular interactions.</b> 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		
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	2	

	particle in the box. Related chemical problems. Rotor and oscillator models. The elements of spectroscopy.	
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	2
	distribution and basic information about systems.	
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	N1 Lecture			
N2	Problems solving			
N3	N3 Project preparation			

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

F1	PEK_Cl01-	Electronic test
	PEK_Cl08	
F2	PEK_La1-	Projects
	PEK_La15	

### **PRIMARY LITERATURE:**

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

### **SECONDARY LITERATURE:**

- [40] L. Piela, Idee Chemii Kwantowej, PWN, Warszawa, 2010.
- [41] W. Kołos, Chemia Kwantowa, PWN, Warszawa, 1975.
- [42] K. Pigoń, Z. Ruziewicz, Chemia Fizyczna (cz. 2), PWN, Warszawa, 2005.
- [43] 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,	C3	Wy10	N1

	S2Ach1_W06, S2Ach4_W06			
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