

Faculty of Chemistry					
SUBJECT CARD					
Name of subject in Polish	Modelowanie molekularne				
Name of subject in English	Molecular modeling				
Main field of study (if applicable):	Biotechnology, Chemistry				
Specialization (if applicable):	Bioinformatics, Medicinal Chemistry				
Profile:	academic				
Level and form of studies:	2nd level, full-time				
Kind of subject:	obligatory				
Subject code					
Group of courses	NO				
	Lecture	Classes	Laboratory	Project	Seminar (spec. BII)
Number of hours of organized classes in University (ZZU)	15		30		15
Number of hours of total student workload (CNPS)	60		60		30
Form of crediting	Examination		crediting with grade		crediting with grade
For group of courses mark final course with (X)					
Number of ECTS points	2		2		1
including number of ECTS points for practical (P) classes			2		1
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	0,65		1,4		0,7
PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES					
Basic knowledge of atomic and molecular structure concepts					
Basic knowledge of analytic geometry					
Basic knowledge of computer science					
Basic knowledge of organic chemistry					
SUBJECT OBJECTIVES					
C1	Teaching construction of 3-D molecular models				
C2	Teaching applications of quantum chemistry methods				
C3	Teaching elementary concepts of the theory of intermolecular interactions				
C4	Teaching modeling techniques of molecular aggregates				
C5	Teaching modeling chemical reactions				

SUBJECT LEARNING OUTCOMES		
Relating to knowledge:		
PEU_W01 – knowledge of construction of 3-dimensional molecular models and their transformations		
PEU_W02 – knowledge of elementary molecular modeling methods and limits of their applications.		
PEU_W03 – knowledge of major components of intermolecular interaction energy		
PEU_W04 – knowledge of modeling drugs and biocatalysts		
Relating to skills:		
PEU_U01 – ability of construction of 3-D molecular model starting from assumed hybridization type		
PEU_U02 – ability to predict molecular structure and properties		
PEU_U03 – ability to predict possible structures of molecular aggregates		
PEU_U04 – ability to analyse protein-ligand interactions		
PEU_U05 – ability to model dynamic properties of molecular aggregates		
relating to social competences:		
PEU_K01 – ability to comprehend, critically assess and communicate the information from scientific sources related to modeling of biological systems of molecules and their properties.		
PROGRAM CONTENT		
Lectures		Number of hours
Lec 1	Basic concepts. Interdisciplinary character 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
Lec 2	Basic concepts of quantum chemistry. Review of quantum chemistry computational methods. Hueckel Molecular Orbitals and ab initio methods. Theoretical prediction of physical properties and structures.	2
Lec 3	Construction of molecular models – exercises and test	2
Lec 4	Basic concepts of the theory of intermolecular interactions. Perturbation theory. Characteristics of major components of intermolecular interaction components.	2
Lec 5	Hydrogen bonding. Molecular charge distribution and electrostatic models. Force fields.	2
Lec 6	Predicting properties and structure of molecular aggregates – exercises and test.	2
Lec 7	Modeling interactions in receptors and enzyme active centers. Drug design techniques. Molecular dynamics. Homology modeling.	2
Lec 8	Analysis of enzyme catalytic activity and biocatalyst design.	1
	Total hours	15
Laboratory		Number of hours
Lab 1	Introduction and lab organization. Editing of molecular structures.	2
Lab 2	Preparing molecular dynamics simulations	2
Lab 3	Preparing molecular dynamics simulations	2
Lab 4	Analysis of molecular dynamics trajectories	2
Lab 5	Computational task #1.	2
Lab 6	Force field parametrization of arbitral organic molecules: initial topology, atom types and non-bonding parameters	2
Lab 7	Force field parametrization of arbitral organic molecules: optimization of atomic charges	2
Lab 8	Force field parametrization of arbitral organic molecules: bonding parameters	2
Lab 9	Computational task #2.	2
Lab 10	Receptor-ligand docking and virtual screening	2

Lab 11	Quantum mechanical calculation of interaction energies	2
Lab 12	Computational task #3.	2
Lab 13	Introduction to hybrid QM/MM modeling	2
Lab 14	Modeling energy profile of a reaction using QM/MM methods	2
Lab 15	Computational task #4	2
	Total hours	30
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: biocatalyst 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 LEARNING OUTCOMES ACHIEVEMENT		
Evaluation (F – forming (during semester), P – concluding (at semester end))	Learning outcomes number	Way of evaluating learning outcomes achievement
F_Lec1	PEU_W01, PEU_W02, PEU_U01	Test with problem solving
F_Lec2	PEU_W02, PEU_W03, PEU_W04, PEU_U01, PEU_U03	Test with problem solving
C_Lec	PEU_W01, PEU_W02, PEU_W03, PEU_W04, PEU_U01, PEU_U03	F_Lec1+F_Lec2, or final exam (test with problem solving, 24 score points): Score Grade 12-14 3,0 15-16 3,5 17-18 4,0 19-20 4,5 21-22 5,0 23-24 5,5
F_Lab1	PEU_W04, PEU_U05	Computational task #1:
F_Lab2	PEU_W01, PEU_W04, PEU_U01, PEU_U04	Computational task #2
F_Lab3	PEU_W04, PEU_U03, PEU_U04	Computational task #3
F_Lab4	PEU_W04, PEU_U02	Computational task #4
C_Lab	PEU_U01, PEU_U02, PEU_U03, PEU_U04, PEU_U05, PEU_W01, PEUW04	F_Lab1+F_Lab2+F_Lab3+F_Lab4 Total score Grade 14-16 3,0

		17-19 3,5 20-22 4,0 23-25 4,5 26-28 5,0
F_Sem	PEU_K01	Preparation and presentation of seminar on individual topic; Active participation in discussion of presentations of other students
C_Sem	PEU_K01	Final grade
PRIMARY AND SECONDARY LITERATURE		
PRIMARY LITERATURE: [1] L. Piel, Quantum Chemistry Ideas, Elsevier, 2010 [2] A.R. Leach, Molecular Modeling: Principles and Applications, (2-nd Ed), Prentice Hall, 2001 [3] H.D. Hotje, Molecular modeling. Basic principles and applications, (3-rd Ed), Wiley, 2008 [4] T. Schlick, Molecular modeling and simulation, Springer, 2002.		
SECONDARY LITERATURE: [1] F. Jensen, Introduction to computational chemistry, Wiley, 2006 (2-nd Ed) [2] J.M. Goodman, Chemical Applications of Molecular Modeling, RSC, 1999. [3] J.P. Doucet, J. Weber, Computer-Aided Molecular Design, 1996, Academic Press, 1996 [4] G.H. Grant, W.G. Richards, Computational chemistry, Oxford Sci. Publ., 1995		
SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)		
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