Zał. nr 5 do ZW 78/2023

Attachment no. 4. to the Program of Studies

FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in Polish **Modelowanie molekularne**
Name of subject in English **Molecular modeling**
Main field of study (if applicable): **Biosciences**
Specialization (if applicable):
Profile: **academic**
Level and form of studies: **2nd level, full-time**
Kind of subject: **obligatory**
Subject code W03BSS-SM2007W, W03BSS-SM2007L, W03BSS-SM2007S
Group of courses NO

	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)	50		50		25
Form of crediting (Examination / crediting with grade)	Examination		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 classes (P)					
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	1,3		1,4		0,7

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Basic knowledge of atomic and molecular structure concepts
2. Basic knowledge of analytic geometry
3. Basic knowledge of computer science
4. Basic knowledge of organic chemistry

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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 EDUCATIONAL EFFECTS

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 possibile structures of molecular aggregates
PEU_U04 – ability to analyse protein-ligand interactions
PEU_U05 – ability to model dynamic properties of molecular aggregates

PROGRAMME CONTENT

Lecture		Number of hours
Lec 1	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
Lec 2	Basic concepts of quantum chemistry. Review of quantum chemistry computational methods. Hueckel Molecular Orbitals and *ab intio* 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 dynamice. 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	Force field parametrization of arbitral organic molecules: initial topology, atom types and non-bonding parameters	2
Lab 3	Force field parametrization of arbitral organic molecules: optimization of atomic charges	2
Lab 4	Force field parametrization of arbitral organic molecules: bonding parameters	2
Lab 5	Computational task #1.	2
Lab 6	Preparing molecular dynamics simulations	2
Lab 7	Preparing molecular dynamics simulations	2
Lab 8	Analysis of molecular dynamics trajectories	2
Lab 9	Computational task #2.	2
Lab 10	Introduction to hybrid QM/MM modeling	2

Lab 11	Modeling energy profile of a reaction using QM/MM methods	2
Lab 12	Computational task #3.	2
Lab 13	Receptor-ligand docking and virtual screening	2
Lab 14	Quantum mechanical calculation of interaction energies	2
Lab 15	Computational task #4	2
	Total hours	30

Seminar		**Number of hours**
Se1	Student's presentations of selected topics	1
Se2		2
Se3		2
Se4		2
Se5		2
Se6		2
Se7		2
Se8		2
	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 code	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
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
P_lecture = F_Lec1+F_Lec2 or final exam		Score Grade 50-59,99% 3,0 60-69,99% 3,5 70-79,99% 4,0 80-89,99% 4,5 90-100% 5,0
P_lab = F_Lab1+F_Lab2+F_Lab3+F_Lab4		
P_seminar		Preparation and presentation of seminar on individual topic;

	Active participation in discussion of presentations of other students

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] L. Piela, 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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