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 : Dynamika Molekularna
Name of subject in English : Molecular Dynamics
Main field of study (if applicable): Biosciences…….
Specialization (if applicable): Bioinformatics……..
Profile: academic
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code W03BSS-SM2002W, W03BSS-SM2002L
Group of courses NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30		30		
Number of hours of total student workload (CNPS)	100		50		
Form of crediting (Examination / crediting with grade)	Crediting with grade		Crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	4		2		
including number of ECTS points for practical classes (P)			2		
including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU)	1,3		1,4		

*delete as not necessary

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. General Chemistry, Physics I and I
2. Algebra, Mathematical Analysis
3. Physical Chemistry

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SUBJECT OBJECTIVES

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

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:

PEU_W01 – Basic concepts and laws of statistical thermodynamics
PEU_W02 – Potential energy form for a force field and understanding the physical meaning of each term
PEU_W03 – Methods to search for a global minimum in biological systems
PEU_W04 – How to choose suitable algorithms for molecular dynamics simulations
PEU_W05 – Algorithms to control temperature and pressure
PEU_W06 – Algorithms to calculate free energy within molecular dynamics framework
PEU_W07 – Analysis of MD results

Relating to skills:

PEU_U01 – Practical knowledge of Linux operating sytem
PEU_U02 – Practical knowledge of specific software to visualize and manipulate biomolecules
PEU_U03 – Practical knowledge of preparing input files and run and analyze simple minimization and MD simulations
PEU_U04 – Practical knowledge on how to prepare and run basic MD simulations for proteins

Relating to social competences:

PEU_K01 student is ready to critically evaluate his/her knowledge and received content

PROGRAMME CONTENT

Lectures		Nu
Lec 1	**Basic concepts.** Molecular mechanics vs. quantum mechanics. Limitations of molecular mechanics. How good can MD be? - comparison with experimental results. The choice of a time step in MD simulations to describe various phenomena.	2
Lec 2	**Introduction to statistical thermodynamics.** Permutations and configurations. Probability theory in chemistry. Stirling approximation. Maxwell distribution. Partition function. Significance of Boltzmann distribution in chemistry. Statistical ensembles. Canonical ensemble. Canonical partition function: translational, rotational, vibrational and electronic terms.	2
Lec 3	**Introduction to statistical thermodynamics – part 2.** Internal energy and partition function: translational, rotational, vibrational and electronic contributions. Heat capacity and partition function.Entropy and partition function. Boltzmann equation and canonical partition function. Residual entropy. Free energy and equilibrium constant and partition function.	2
Lec 4	**Quiz 1.** Statistical thermodynamics	2
Lec 5	**Force field – part 1.** Definition of force field. Potential energy in force field. Bonding and non-bonding terms of potential. Harmonic and Morse potential. Mixed terms. Point charge model. RESP procedure. Buckingham and Lennarda-Jones potentials. Combination rules to create van der Waals parameters. Scaling of non-bonding potentials. Evaluation of cpu time in calculations of various potential energy terms.	2
Lec 6	**Force field – part 2.** All-atom and united-atom force fields. Transferability of force field parameters among different force fields. Accuracy of various force fields.	2
Lec 7	**Preparation of input files for MD simulations.** GROMACS options. How to choose an initial structure? A choice of a force field. Phases of MD procedure: minimization, heating, equilibration and production phase.Preparation of all required input files for MD simulations.	2

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

Computer laboratory	Nu

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

TEACHING TOOLS USED	
N1	Lecture with multimedia presentation

N2	Solving pratice problem sets
N3	Usage of software
N4	Preparation of reports

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1	PEU_W01, PEU_K01	Quiz 1
F2	PEU_W02 – PEU_W07, PEU_K01	Quiz 2
P (laboratory)	PEU_U01 – PEU_U05	Report+obligatory presence at all laboratory classes
P (lecture) = 3.0 if (F1 + F2) = 50-60% max. no of poins **3.5 if (F1 + F2) = 61-70% max. no of poins** **4.0 if (F1 + F2) = 71-80% max. no of poins** **4.5 if (F1 + F2) = 81-90% max. no of poins** **5.0 if (F1 + F2) = 91-99% max. no of poins** **5.5 if (F1 + F2) = 100% max. no of poins.**		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1]. D. Frenkel, B. Smith “Understanding Molecular Simulation”, Academic Press, 2001.

[2] J.M. Haile “Molecular Dynamics Simulation: Elementary Methods”, Wiley-Interscience, 1997.

SECONDARY LITERATURE:

[1**]** M. P. Allen, D. J. Tildesley “Computer Simulation of Liquids”, Oxford University Press, 1989.

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