

Faculty of Chemistry					
SUBJECT CARD					
Name of subject in English:	Molecular dynamics				
Main field of study (if applicable):	Biotechnology				
Specialization (if applicable):	Bioinformatics				
Profile:	academic				
Level and form of studies:	2nd level, full-time				
Kind of subject:	obligatory				
Subject code:	CHC024052				
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)	120		60		
Form of crediting	crediting with grade		crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	4		2		
including number of ECTS points for practical (P) classes			2		
including number of ECTS points for direct teacher-student contact (BK) classes	1		1		
PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES					
1. General Chemistry, Physics I and II					
2. Algebra, Mathematical Analysis					
3. Physical Chemistry					
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		
<p>relating to knowledge: PEK_W01 – Basic concepts and laws of statistical thermodynamics PEK_W02 – Potential energy form for a force field and understanding the physical meaning of each term PEK_W03 – Methods to search for a global minimum in biological systems PEK_W04 – How to choose suitable algorithms for molecular dynamics simulations PEK_W05 – Algorithms to control temperature and pressure PEK_W06 – Algorithms to calculate free energy within molecular dynamics framework PEK_W07 – Analysis of MD results</p> <p>Relating to skills:</p> <p>PEK_U01 – Practical knowledge of Linux operating system PEK_U02 – Practical knowledge of specific software to visualize and manipulate biomolecules PEK_U03 – Practical knowledge of preparing input files and run and analyze simple minimization and MD simulations PEK_U04 – Practical knowledge on how to prepare and run basic MD simulations for proteins</p> <p>Relating to social competences: PEK_K01 student is ready to critically evaluate his/her knowledge and received content</p>		
PROGRAMME CONTENT		
Lectures		Number of hours
Lec 1	Basic concepts. Molecular mechanics vs. quantum mechanics. Limitations of molecular mechanics. How good can MD be? - comparison with experimental results. The choice of a time step in MD simulations to describe various phenomena.	2
Lec 2	Introduction to statistical thermodynamics. Permutations and configurations. Probability theory in chemistry. Stirling approximation. Maxwell distribution. Partition function. Significance of Boltzmann distribution in chemistry. Statistical ensembles. Canonical ensemble. Canonical partition function: translational, rotational, vibrational and electronic terms.	2
Lec 3	Introduction to statistical thermodynamics – part 2. Internal energy and partition function: translational, rotational, vibrational and electronic contributions. Heat capacity and partition function. Entropy and partition function. Boltzmann equation and canonical partition function. Residual entropy. Free energy and equilibrium constant and partition function.	2
Lec 4	Quiz 1. Statistical thermodynamics	2

Lec 5	Force field – part 1. Definition of force field. Potential energy in force field. Bonding and non-bonding terms of potential. Harmonic and Morse potential. Mixed terms. Point charge model. RESP procedure. Buckingham and Lennarda-Jones potentials. Combination rules to create van der Waals parameters. Scaling of non-bonding potentials. Evaluation of cpu time in calculations of various potential energy terms.	2
Lec 6	Force field – part 2. All-atom and united-atom force fields. Transferability of force field parameters among different force fields. Accuracy of various force fields.	2
Lec 7	Preparation of input files for MD simulations. GROMACS options. How to choose an initial structure? A choice of a force field. Phases of MD procedure: minimization, heating, equilibration and production phase. Preparation of all required input files for MD simulations.	2
Lec 8	Methods of searching for global minimum in biomolecules. Methods for energy minimization. Levinthal paradox. Local and global minima in biosystems. Monte-Carlo method. Simulated annealing method. Genetic algorithm. Chain growth method. Homology modelling. Distance-geometry algorithm. 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		Number of hours
Lab 1	Requirements to pass a laboratory course.	2
Lab 2	Basic Linux commands	2
Lab 3	Basic commands of '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 practice problem sets	
N3	Usage of software	
N4	Preparation of reports	

EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT		
Evaluation F – forming (during semester), C – concluding (at semester end)	Educational effect number	Way of evaluating educational effect achievement
F1	PEK_W01	Quiz 1
F2	PEK_W02 – PEK_W07	Quiz 2
P (laboratory)	PEK_U01 –PEK_U05	Report+obligatory presence at all laboratory classes
<p>P (lecture) = 3.0 if (F1 + F2) = 50-60% max. no of points 3.5 if (F1 + F2) = 61-70% max. no of points 4.0 if (F1 + F2) = 71-80% max. no of points 4.5 if (F1 + F2) = 81-90% max. no of points 5.0 if (F1 + F2) = 91-99% max. no of points 5.5 if (F1 + F2) = 100% max. no of points.</p>		
PRIMARY AND SECONDARY LITERATURE		
<p><u>PRIMARY LITERATURE:</u> [1]. D. Frenkel, B. Smith “Understanding Molecular Simulation”, Academic Press, 2001. [2] J.M. Haile “Molecular Dynamics Simulation: Elementary Methods”, Wiley-Interscience, 1997.</p> <p><u>SECONDARY LITERATURE:</u> [1] M. P. Allen, D. J. Tildesley “Computer Simulation of Liquids”, Oxford University Press, 1989.</p>		
SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)		
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