BIOTECH-10:	**MOLECULAR MODELLING**
GENERAL INFORMATION	
Course Coordinator(s)	Hrvoje Brkić, PhD, Assist. prof.
Associate(s)	Dario Faj, PhD, Full prof.
Study Programme	Interdisciplinary Graduate Study Programme in English: Biotechnology
Course Status	Obligatory
Year of Study, Semester	1st Year / 2nd Semester
Credits (ECTS)	**3**
Teaching Method (number of classes)	Lectures: 30 ; Seminars: 15 ; Exercises: -
Expected Number of Students in the Course	25-30
COURSE DESCRIPTION	
Course Aims	
Provide students with elementary of molecular modeling and usage of molecular modeling in biotechnology. Besides this students are going to be able to understand biophysical principles used in molecular modeling and in this way level up the knowledge about molecular modeling above just using bioinformatics tools. Students are going to be provided with sufficient amount of theoretical knowledge that is going to be used in choosing the method of molecular modeling in development of new bio-active molecules.	
Prerequisites for Enrolment and the Entry Competencies Required for the Course	
Completed undergraduate university study programme from the area of natural sciences (chemistry, biology) or biotechnical sciences, or biomedicine and healthcare.	
Learning Outcomes at the Programme Level Contributed by the Course	
BIOTECH-9; INDBIOT-1; INDBIOT-5; MEDBIOT-2; MEDBIOT-3; MEDBIOT-4	
Learning Outcomes at the Course Level	
After completing the course, the student will be able to: 1. Understand how quantum mechanical calculations are used to describe chemical reactions. 2. Understand what approximations are used by semi-empirical calculations, and for what they are most commonly used. 3. Understand the methods of molecular mechanics and molecular dynamics, and know in which situations they can be applied. 4. Explain which approximations are used in molecular modelling and what are the advantages and disadvantages of each approximation 5. Use software packages and parameterize the system in the force field 6. Perform a simple protein simulation analysis 7. Graph the results of molecular dynamics and the resulting molecular structures	
Course Content	
Lectures. Useful concepts of molecular modelling. Coordinate systems, potential energy surfaces, computer hardware and software applicable in modelling. Mathematical concepts. Introduction to Computer Quantum Mechanics. Single-electron atoms, multi-electron atoms and molecules. Base sets, *ab initio* accounts. Empirical force fields, Molecular mechanics. General properties of molecular mechanics, bond elongation, bending angles, electrostatic interactions, van der Waals interactions, nonbonding interactions, hydrogen bonds in molecular mechanics, force fields. Energy minimization and related methods for free energy surface research. First degree minimization, conjugate gradients, steepest descent method. **Seminars.** Computer simulation methods. Phase space, calculation of simple thermodynamic parameters, boundary conditions. Basics of Statistical Mechanics. Molecular dynamics simulations. Topologies, simulations by simple methods, limitations in molecular dynamics. Conformational changes. Monte Carlo simulation methods. Statistical checks and variance reduction.	

Processing and displaying results. Graphical representation of time-dependent parameters, three-dimensional representation of structures and chemical interactions over time.

Teaching Methods

Lectures; seminars;

Students' Obligations

Attendance at all forms of classes is mandatory and the students are obligated to attend all knowledge tests. The students may be absent from 30% (full-time students) and 50% (part-time students) of each of the forms of classes, provided that the absence is justified. An exercise or a seminar which has not been completed must be made up through a midterm exam.

Monitoring the Activity of the Students *(Connecting Learning Outcomes, Teaching Methods, and Grading)*

Class-related activity	ECTS	Learning outcome	Student activity	Evaluation method	Grade points	
					Min.	Max.
Attending classes (lectures) Seminar work	0,2 1,8	1-7 4,6,7	Attendance at classes, and laboratory Seminar work	Keeping records Presentation of seminar work	1 29	5 45
Final exam	1	1-7	Studying for the final exam	Written exam	30	50
Total	**3**				**50**	**100**

Evaluation of the written part of the final exam

Percentage of correct answers (%)	Grade
>95.00	50
90.00-94.99	47
85.00-89.99	45
80.00-84.99	40
75.00-79.99	38
70.00-74.99	35
65.00-69.99	33
60.00-64.99	30

Forming the final grade:
The points granted for the final exam are added to the grade points awarded during class attendance. The grading process is conducted by absolute distribution, i.e. based on total achievements, and compared to the numerical system in the following manner:
A – Excellent (5): 90-100 grade points; B – Very Good (4): 80-89.99 grade points; C – Good (3): 65-79.99 grade points; D – sufficient (2): 50-64.99 grade points.

Mandatory Literature (available in the library and via other media)

Title	Number of copies in the library	Availability via other media
Andrew R. Leach Molecular Modelling Principles and applications (2nd Ed.) Pearson Education Limited, 2001.	1	

Additional Literature

Cullity and Stock: Elements of X-ray diffraction (3rd Ed.) Pretience and Hall, 2001.
Quality Assurance Procedures Designed to Ensure the Acquisition of Outcomes and Competencies
Anonymous, quantitative, standardised student survey on the course and the teacher's work implemented by the Quality improvement office of the Faculty of Medicine Osijek and/or the Faculty of Food Technology Osijek.
Note
E-learning is not included in the class quota, but it is used in teaching and it contains links to various sites and video and audio materials available on websites.