School of Engineering and Natural Sciences / Biomedical Engineering (English)

2024 - 2025 Academic Year

INTRODUCTION to COMPUTATIONAL BIOPHYSICS

Syllabus

Course Description					
Name	**Code**	**Semester**	**T+A Hour**	**Credit**	**ECTS**
INTRODUCTION to COMPUTATIONAL BIOPHYSICS	BME3249570	Spring Semester	3+0	3	6

Prerequisites Courses	
Recommended Elective Courses	
Language of Instruction	English
Course Level	First Cycle (Bachelor's Degree)
Course Type	Elective
Course Coordinator	Assoc.Prof. Özge ŞENSOY
Name of Lecturer(s)	Assoc.Prof. Özge ŞENSOY
Assistant(s)	
Aim	It is aimed to teach the students some widely-used computational techniques such as molecular modeling, molecular docking and molecular dynamics simulations along with the parameters used to optimize simulations.
Course Content	This course contains; Introduction to Quantum Chemistry,An overview to the Quantum Chemical Methods,Introduction to Statistical Mechanics,Molecular Dynamics,Force Fields,Solvation Models,Electrostatics in Molecular dynamics,Free Energy Calculations,Enhanced Sampling Techniques,Hybrid Simulation Methods : QM/MM calculations,Coarse Grained Potentials ,Molecular Docking,Application of above-mentioned techniques to biological problems -I,Application of above-mentioned techniques to biological problems -II.

Course Learning Outcomes	**Teaching Methods**	**Assessment Methods**
Different aspects between molecular mechanics and quantum mechanics are described on a comparative basis.	10, 12, 13, 20, 21, 3, 4	F
Different force-fields and water models can be analzyed on a comparative basis.	10, 12, 13, 14, 21, 3, 4	
Simulations can be performed using parallel-computing systems.	21, 6	
Molecular dynamics simulations are performed and the results are analzyed.	11, 13, 21	

Teaching Methods	10: Discussion Method, 11: Demonstration Method, 12: Problem Solving Method, 13: Case Study Method, 14: Self Study Method, 20: Reverse Brainstorming Technique, 21: Simulation Technique, 3: Problem Baded Learning Model, 4: Inquiry-Based Learning, 6: Experiential Learning
Assessment Methods	F: Project Task

Lecture Schedule

Sequence	**Topics**	**Preliminary Preparation**
1	Introduction to Quantum Chemistry	
2	An overview to the Quantum Chemical Methods	
3	Introduction to Statistical Mechanics	
4	Molecular Dynamics	
5	Force Fields	
6	Solvation Models	
7	Electrostatics in Molecular dynamics	
8	Free Energy Calculations	
9	Enhanced Sampling Techniques	
10	Hybrid Simulation Methods : QM/MM calculations	
11	Coarse Grained Potentials	
12	Molecular Docking	
13	Application of above-mentioned techniques to biological problems -I	
14	Application of above-mentioned techniques to biological problems -II	

Evaluation Methods	**Weight(%)**
Midterm Exam	30
General Exam	70

Resources
Frenkel and Smit, Understanding Molecular Simulation : From Algorithms to Applications, , Academic Press, Computational Science Series Sunum