Course Syllabus

Code - Course Title	**FKM534 - Molecular Docking and Dynamics Simulation in Medicinal Chemi**
Course Type	II. SEMESTER
Laboratory + Practice	3+0
ECTS	**6.0**
Language of Instruction	Türkçe
Course Type	Elective Courses
Course Instructor(s)	DOÇ. DR. BEGÜM NURPELİN SAĞLIK ÖZKAN

Mode of Delivery	Face to face learning
Prerequisites	There is no prerequisite or co-requisite for this course.
Courses Recomended	There is no recommended optional program component for this course.
Recommended Resources	There is no recommended or required reading for this course.
Work Placement	Work placement is not applicable.

Course Syllabus

Weeks	Learning Outcomes	Topics	Teaching Methods
Week - 1		Introduction to molecular modeling	
Week - 2		Molecular modeling approaches	
Week - 3		Molecular modeling applications and examples in drug design	
Week - 4		Identification and use of programs used in medicinal chemistry	
Week - 5		2-Dimensional and 3-dimensional representation of chemical compounds	
Week - 6		Studies on protein database and representation of proteins	
Week - 7		Preliminary studies for molecular docking	
Week - 8		Molecular docking studies	
Week - 9		Evaluation of molecular docking studies	
Week - 10		Use of molecular dynamics programs in drug development	
Week - 11		Preliminary studies for molecular dynamics simulation	
Week - 12		Molecular dynamics simulations	
Week - 13		Evaluation of molecular dynamics simulations	

Course Syllabus

Weeks	Learning Outcomes	Topics	Teaching Methods
Week - 14		Applications for molecular docking and dynamics simulation	

Learning Outcomes

#	Learning Outcome
1	Learns the basic information to be used in computer applications in medicinal chemistry.
2	Gains basic knowledge of medicinal chemistry in drug active ingredient development studies.
3	Examines drug-enzyme interactions.
4	Learns conformational analysis.
5	Analyzes receptor-substrate modeling.
6	Establishes a computer-assisted connection between the structures of drug active ingredients and their possible biological activities.
7	Establishes a computer-assisted connection between the structures of drug active ingredients and their possible biological activities.
8	Learns computer aided drug design methods.
9	Gains knowledge of new drug active ingredient design, quantitative structure-effect relationships and computer applications in this process.
10	Obtains information about the statistical evaluation of the results of quantitative and biological analysis of drug active ingredients.
11	Conducts molecular docking studies and analyzess related results.
12	Experiences molecular dynamics simulation and analyzes relevant results.

Sustainable Development Goals

No content has been provided.

Course Theme

No content has been provided.

AKTS Workload

Activity	Duration (Hour)	Count	Workload
Teorik Derse Katılım	0	0	0
Sınıf Dışı Çalışma (Ön Hazırlık & Pekiştirme Amaçlı)	0	0	0
Ödevler	0	0	0
Proje - Rapor - Sunum Hazırlama	0	0	0
Ara Sınav Hazırlığı (sınav süresi dahil)	0	0	0
Final Sınavı Hazırlığı (sınav süresi dahil)	0	0	0
Uygulama (Laboratuvar, Müzik/Enstrüman Uygulaması, Atölye/Saha Çalışması vb.)	0	0	0
Staj Uygulaması	0	0	0
		Calculated ECTS	**0**

Assessment Method and Passing Requirements

No content has been provided.