Course Syllabus

Code - Course Title	**FKM629 - Molecular Modelling in Drug Research**
Course Type	II. SEMESTER
Laboratory + Practice	3+0
ECTS	**7.5**
Language of Instruction	Türkçe
Course Type	Elective Courses
Course Instructor(s)	DOÇ. DR. ASAF EVRİM EVREN

Mode of Delivery	The mode of delivery of this course is Face to face
Prerequisites	The students who selected this course should take and pass the Pharmaceutical Chemistry (at least -I, -II) courses on Pharmacy Training Programme and should know the concept of structure-activity, should know and use effectively 2- and 3-D Chemical Draw Programmes
Courses Recomended	Students who take this course should have taken at least ECZ301-Pharmaceutical Chemistry I and ECZ302-Pharmaceutical Chemistry II courses.
Recommended Resources	- All scientific articles/papers related to topics on Molecular Modelling in Drug Research (via SciFinder and Web of Science)- MOE software package (https://www.chemcomp.com) - Schrodinger Training suites (https://www.schrodinger.com)- Merck Index- RxMediaPharma® 2018 Interactive Drug Information Source, General Editor: Prof. Dr. Levent Üstünes.
Work Placement	Lessons are limited because of the fact that after the basic information is given in the first weeks, it is done practically at the computer. It is recommended that students have portable computers. It is expected that they will be able to download some free programs to their computers and research on them.

Course Syllabus

Weeks	Learning Outcomes	Topics	Teaching Methods
Week - 1		Computer techniques for development and optimization of “Leading structure” on the drug researches	
Week - 2		Computer techniques for development and optimization of “Leading structure” on the drug researches	
Week - 3		Molecular modelling	
Week - 4		Molecular imaging programmes	
Week - 5		Molecular imaging programmes	
Week - 6		Molecular model design via mathematical methods	
Week - 7		Recognition of interactions between molecules	
Week - 8		Simulation techniques (Molecular Dinamic)	
Week - 9		simulation techniques (Monte Carlo)	

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Weeks	Learning Outcomes	Topics	Teaching Methods
Week - 10		Simülasyon teknikleri (Enerji minimizasyonu)	
Week - 11		Comparative modelling	
Week - 12		Drug design	
Week - 13		Drug design	
Week - 14		Chemoinformatics	

Learning Outcomes

#	Learning Outcome
1	Will be able to optimize to develop lead structure in drug research
2	Will be able to explain molecular modeling
3	Will be able to use package programs developed for the display of molecules
4	Will be able to design and adapt modeling at the molecular level with mathematical methods
5	Will be able to compare intermolecular interactions
6	Will be able to describe simulation techniques (Molecular Dynamics, Monte Carlo, energy minimization)
7	Will be able to develop and improve comparative modeling
8	Will be able to suggest drug design
9	Will be able to distinguish chemoinformatic methods

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

AKTS Workload

Activity	Duration (Hour)	Count	Workload
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.