

Import module

[E1.21]	Computational Drug Design	Compulsory elective module	5 CP (total) = 150 h				4 SWS	
			Contact hours 4 SWS / 60 h	Independent study 90 h				
Content								
	<p><u>Lecture</u>: The theory and application of computational methods used in drug design and discovery are presented in an application-oriented way. For this purpose, different computational methods, such as docking, modeling, ligand-based approaches, bioinformatic approaches as well as molecular dynamics (MD) simulation-based methods, are introduced. Their applications in drug design will be discussed with numerous examples from published scientific literature. Furthermore, for each method the widely used softwares will be introduced and exercises utilising these software are integrated into the lectures.</p> <p><u>Practical course</u>: During the practical part, the individual methods are applied to simple problems of drug design. The topics offer a wide variety of computational methods spanning theoretical biophysics, biochemistry, and medicinal chemistry.</p>							
Learning outcomes and skills								
	The goal of this module is to introduce the students to the modern computational tools widely used for drug design. Students understand the theory, application, and limitations of each method and would be able to use them for specific projects. Through the focus on sample programs, students learn how to use computational methods in different projects.							
Admissions requirements/Conditions for participation in the module/courses								
	None							
Recommended prior knowledge								
	Basic knowledge of programming and Linux environment, bachelor-level knowledge of organic chemistry as well as good knowledge of protein chemistry and structure. Use your own laptop during the lecture.							
Organizational details								
	Import module, the registration and cancellation deadlines of the Bachelor's/Master's Biophysics regulations apply. (The exam requires online registration , no later than seven days before the exam date. You can withdraw up to one working day before the exam date without giving reasons.)							
Module allocation (degree programme/faculty)			Master Biophysics / FB13					
Eligibility of the module for other courses			Master Biochemistry / FB14					
Module offered			winter semester					
Duration			1 semester					
Module coordinator			Prof Hummer					
Course requirements for credits								
Participation record								
Coursework			Lecture: Written (exam, 90 min.) or expert discussion (30 min.)					
Forms of teaching / learning			Lecture, practical course					
Language teaching and instruction			English					
Module assessment			Form / duration / content, if applicable					
Final module assessment			None					
Cumulative module assessment consisting of								
Composition of the module grade for cumulative module assessment								
			Mode of teaching / study	Semester hours per week	Semester CP			
					1	2	3	4
	Computational drug design		L	2	3			
	Computational drug design		P	2	2			
	TOTAL			4	5			