

COURSE DESCRIPTION

Academic year: 2026/2027	
University: Comenius University Bratislava	
Faculty: Faculty of Pharmacy	
Course ID: FaF.KChTL/10-Mgr-A/26	Course title: Principles of Molecular Modelling
Educational activities: Type of activities: practicals / lecture Number of hours: per week: 2 / 1 per level/semester: 28 / 14 Form of the course: on-site learning	
Number of credits: 2	
Recommended semester: 4.	
Educational level: I.II.	
Prerequisites:	
Course requirements: preliminary evaluation: project elaboration from practicals final evaluation: final test A: 92,00 % – 100,00 %; B: 84,00 % – 91,99 %; C: 76,00 % – 83,99 %; D: 68,00 % – 75,99 %; E: 60,00 % – 67,99 %; Fx: 0,00 - 59,99 %. Scale of assessment (preliminary/final): 40/60	
Learning outcomes: The course should educate the students about the basic principles of computer chemistry and the methods of computer aided molecular design.	
Class syllabus: To master the subject Principles of Molecular Modeling at a sufficient level, knowledge of the subject Organic Chemistry 1 is required. The students work with the programs available at the Department of Chemical Theory of Drugs – Alchemy, Chemwind or Chems sketch, Rasmol, MS Word, with the use of the internet network and available databases (PDB). Primarily students work on the tasks on molecules designed as potential drugs, such as finding the optimal conformation of the molecule, electron distribution in the molecule, the relationship between the structure and properties. They learn how to browse the PDB database and the principle of docking of molecules in enzyme active site. During the tuition students will elaborate their given project, each on their own molecule.	
Recommended literature: Alan Hinchliffe : Molecular Modeling for Beginners, Wiley, 2003.	
Languages necessary to complete the course: English language	
Notes: The course is held only in summer semester. Minimum of 2 students must be signed up for the course to take place.	

Past grade distribution						
Total number of evaluated students: 0						
A	ABS	B	C	D	E	FX
0,0	0,0	0,0	0,0	0,0	0,0	0,0
Lecturers: Mgr. Lucia Lintnerová, PhD., doc. Ing. Martin Pisárčík, CSc., Mgr. Peter Herich, PhD.						
Last change: 11.06.2026						
Approved by: prof. PharmDr. Ján Klimas, PhD., MPH						