

Subject card

Subject name and code	Computationally Added Drug Design, PG_00117802						
Field of study	Chemistry						
Date of commencement of studies	October 2026	Academic year of realisation of subject				2027/2028	
Education level	Master's studies	Subject group				Optional subject group	
Mode of study	full-time studies	Mode of delivery				at the university	
Year of study	2	Language of instruction				English	
Semester of study	4	ECTS credits				2.0	
Learning profile	academic	Assessment form				credit	
Conducting unit	Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		dr inż. Karolina Jagiełło				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	30.0	0.0	0.0	30
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours		Self-study	SUM
	Number of study hours	30		5.0		15.0	50
Subject objectives	Developing skills in planning the strategies of computationally added drug design						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student knows the possibilities and limitations of computational methods utilized in drug design.	[SW2] presentation/project/paper/report
	[CHEMMU2_U03] Finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry.	The student: understands risks and benefits related to the use of computational methods in the process of drug design; formulates his/her opinions based on a solid scientific background	[SU1] oral statement/conversation/discussion
	[CHEMMU2_K03] Understands the need for systematic work on various projects of a long-term nature and knows how to set priorities for the implementation of undertaken tasks.	The student: provides examples of computational methods used in drug design, proposed (selects) appropriate computational drug design strategies	[SK1] oral statement/conversation/discussion
	[CHEMMU2_K04] Correctly identifies and resolves dilemmas related to the profession of a chemist.	The student: provides examples of computational methods used in drug design, proposed (selects) appropriate computational drug design strategies	[SK1] oral statement/conversation/discussion
	[CHEMMU2_U01] Plans and implements chemical experiments of medium complexity.	The student: understands risks and benefits related to the use of computational methods in the process of drug design; formulates his/her opinions based on a solid scientific background	[SU1] oral statement/conversation/discussion
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	The student knows the possibilities and limitations of computational methods utilized in drug design.	[SW2] presentation/project/paper/report
[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	The student knows the possibilities and limitations of computational methods utilized in drug design.	[SW1] oral statement/conversation/discussion [SW2] presentation/project/paper/report	
Subject contents	Fragment-based drug discovery. Receptor-based drug discovery. Sequence-based drug discovery. Conformation-based drug discovery. High throughput virtual screening. Hit identification. Hit-to-lead optimization. Prediction of ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) properties.		
Prerequisites and co-requisites			
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Written report	51.0%	100.0%
Recommended reading	Basic literature	Scientific publication	
	Supplementary literature	Scientific publication	
	eResources addresses		
Example issues/ example questions/ tasks being completed			
Work placement	Not applicable		

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