University of Gdańsk

Subject card

Subject name and code	Computationally Added Drug Design, PG_00117802		
Field of study	Chemistry		
Date of commencement of studies	October 2024	Academic year of realisation of subject	2025/2026
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 english
Semester of study	4	ECTS credits	2.0
Learning profile	academic	Assessment form	
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

<table>
<tr><td>Learning outcomes</td><td>
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<tr><th>Course outcome</th><th>Subject outcome</th><th>Method of verification</th></tr>
<tr><td>[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.</td><td>The student knows the possibilities and limitations of computational methods utilized in drug design.</td><td>[SW2] presentation/project/paper/ report</td></tr>
<tr><td>[CHEMMU2_U03] Finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry.</td><td>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</td><td>[SU1] oral statement/conversation/ discussion</td></tr>
<tr><td>[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.</td><td>The student:
provides examples of computational methods used in drug design,
proposed (selects) appropriate computational drug design strategies</td><td>[SK1] oral statement/conversation/ discussion</td></tr>
<tr><td>[CHEMMU2_K04] Correctly identifies and resolves dilemmas related to the profession of a chemist.</td><td>The student:
provides examples of computational methods used in drug design,
proposed (selects) appropriate computational drug design strategies</td><td>[SK1] oral statement/conversation/ discussion</td></tr>
<tr><td>[CHEMMU2_U01] Plans and implements chemical experiments of medium complexity.</td><td>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</td><td>[SU1] oral statement/conversation/ discussion</td></tr>
<tr><td>[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.</td><td>The student knows the possibilities and limitations of computational methods utilized in drug design.</td><td>[SW2] presentation/project/paper/ report</td></tr>
<tr><td>[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.</td><td>The student knows the possibilities and limitations of computational methods utilized in drug design.</td><td>[SW1] oral statement/ conversation/discussion
[SW2] presentation/project/paper/ report</td></tr>
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<tr><td>Subject contents</td><td>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.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td></td></tr>
<tr><td>Assessment methods and criteria</td><td>
<table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Written report</td><td>51.0%</td><td>100.0%</td></tr>
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<tr><td>Recommended reading</td><td>
<table>
<tr><td>Basic literature</td><td>Scientific publication</td></tr>
<tr><td>Supplementary literature</td><td>Scientific publication</td></tr>
<tr><td>eResources addresses</td><td>Adresy na platformie eNauczanie:</td></tr>
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<tr><td>Example issues/ example questions/ tasks being completed</td><td></td></tr>
<tr><td>Work placement</td><td>Not applicable</td></tr>
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