GDAŃSK UNIVERSITY
OF TECHNOLOGY

Subject card

Subject name and code	Modern applications of artificial intelligence in biomolecule modeling, PG_00072664		
Field of study	Chemical Technology, Chemistry, Biotechnology, Engineering and Technologies of Energy Carriers, Corrosion , Green Technologies, InfoBioChem		
Date of commencement of studies	February 2026	Academic year of realisation of subject	2026/2027
Education level	second-cycle studies	Subject group	
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish
Semester of study	2	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. inż. Jacek Czub	
	Teachers		

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	30.0	0.0	0.0	45
	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	45	5.0	10.0	60

Subject objectives	The subject aims to present and provide a practical introduction to artificial intelligence tools currently developed and used in structural bioinformatics and computational chemistry. Students will understand the basic principles of deep-learning algorithms behind the success of tools such as AlphaFold and RoseTTAFold, become familiar with the concepts of inverse folding and protein inpainting, learn about foundation models enabling representation of biomolecules, small molecules and genomes, and use interactive notebooks and servers to apply available tools in practice.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_W01] recognizes problems of modern chemistry, including properties and obtaining chemical compounds, necessary for making calculations, including the dependence of the compound's structure and its reactivity	knows and identifies contemporary research problems in structural bioinformatics and computational chemistry that can be addressed using AI methods; explains relationships between molecular sequence, structure, stability, reactivity and interactions and the results generated by tools such as AlphaFold, RoseTTAFold, inverse-folding/inpainting methods and neural potentials.	[SW1] Assessment of factual knowledge
[K7_W03] recognizes and describes phenomena in the field of physics, including elements of quantum mechanics, solid state physics and nuclear physics, necessary to predict the course of physical phenomena and to solve technical problems	has the necessary knowledge to explain the physical principles and limitations of AI methods used to model biomolecular structures, conformers, intermolecular interactions and molecular energetics; interprets these results in relation to classical and quantum descriptions of molecular systems.	[SW1] Assessment of factual knowledge
[K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation	prepares a technical/scientific report and a short presentation documenting the results of mini-projects; uses text, tables, plots and molecular-structure visualisations to present input data, applied methods, results and limitations of AI tools for biomolecular modelling.	[SU1] Assessment of task fulfilment [SU5] Assessment of ability to present the results of task
[K7_U01] integrates and interprets information from literature, databases and other sources	collects, integrates and interprets information from scientific literature, structural, sequence and chemical databases, and online AI servers; prepares input data, assesses the credibility of outputs and draws conclusions from model predictions within mini-projects.	[SU1] Assessment of task fulfilment [SU5] Assessment of ability to present the results of task [SU2] Assessment of ability to analyse information

Subject contents

Course content – lecture

- The protein-folding problem and the evolution of attempts to solve it: from physics-based approaches to the AlphaFold2 breakthrough and new generative methods using stable diffusion
- The inverse protein-folding problem. Approaches combining simultaneous structure and sequence generation
- Prediction of structures and conformers for nucleic acids, post-translational modifications and small molecules
- Prediction of canonical ensembles of biomacromolecules: going beyond the single-structure paradigm
- Foundation models and representation learning in bioinformatics and cheminformatics
- Application of graph neural networks to predict molecular properties based on 3D structure
- Neural potentials: physical models of molecular energetics trained to accelerate quantum-chemical calculations

Course content – laboratory

- Working with Colab notebooks and graphics processing units
- Minimal basics of the PyTorch library
- Practical discussion of methods for training models and using previously trained models
- Four mini-projects carried out in small groups:

1. Use of servers for protein and nucleic-acid structure prediction, including the effect of point mutations on macromolecular stability
2. Design of protein domains that specifically bind a selected macromolecular target
3. Modern methods of docking and predicting interactions in protein-protein and protein-ligand systems
4. Use and modification of an existing deep-learning architecture to build a predictor of a selected structural property: ion-binding site, ligand-binding pocket or disulfide bridges

Prerequisites and co-requisites

- Knowledge of Python programming
- Knowledge of the conceptual foundations of machine learning and cheminformatics

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Lecture: final test	50.0%	25.0%
Laboratory: four mini-projects (report)	50.0%	75.0%

Recommended reading

Basic literature	Charles Ravarani, Natasha Latysheva: Deep Learning for Biology
Supplementary literature	Simon J.D. Prince: Understanding Deep Learning
eResources addresses	

Example issues/ example questions/ tasks being completed	• How can deep-learning models requiring substantial computational resources be run? • How can a structural model of a protein predicted by a deep-learning algorithm be validated? • Which classes of research problems can currently be addressed using available deep-learning tools? • Which structural and sequence databases can be used to collect input data? How can data be retrieved individually and in batch mode? • Which procedures allow preparation of clean data for training AI models? • Use a selected structure-prediction server to profile protein sensitivity to mutations. • Choose a protein of biomedical importance and design a domain that binds near its active or allosteric site. • Characterise binding of a selected drug to the human hERG protein using docking methods based on stable diffusion. • Carry out, in a group, data cleaning, code modification and training to build a predictive model based on existing graph neural networks.
Practical activites within the subject	Not applicable