GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

| | | | |
|---|---|---|---|
| Subject name and code | Molecular Modelling of Biomolecules, PG_00058279 | | |
| Field of study | Biotechnology | | |
| Date of commencement of studies | February 2024 | Academic year of realisation of subject | 2024/2025 |
| Education level | second-cycle studies | Subject group | Optional subject group |
| Mode of study | Full-time studies | Mode of delivery | at the university |
| Year of study | 1 | Language of instruction | Polish<br>Polish - some materials in English, the software in English |
| Semester of study | 2 | ECTS credits | 2.0 |
| Learning profile | general academic profile | Assessment form | assessment |
| Conducting unit | Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | prof. dr hab. inż. Maciej Bagiński | |
| | Teachers | prof. dr hab. inż. Maciej Bagiński<br>dr inż. Mateusz Kogut | |

**Lesson types and methods of instruction**

| Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
|---|---|---|---|---|---|---|
| Number of study hours | 15.0 | 0.0 | 0.0 | 15.0 | 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 | 2.0 | 18.0 | 50 |

**Subject objectives**

The aim of the course is to familiarize students with selected topics in the field of molecular modeling, which can be useful in carrying out the thesis in the field of drug design and may also serve as the basis for specific items on the third level studies. The strategic objective will be achieved through assimilation of theoretical knowledge as well as practical implementation of tasks in the laboratory.

**Learning outcomes**

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [K7_U07] is able to consider bioethical issues and regulations in research planning and design of biotechnological products and processes | The student understands the basics of drug design, including ethical problems related to drug design. | [SU3] Assessment of ability to use knowledge gained from the subject<br>[SU2] Assessment of ability to analyse information |
| [K7_K02] is aware of the limitations and the necessity of continuous development of knowledge and technology; understands the need for education and constant training | The student understands and is aware of the limitations of molecular modeling methods and the need to educate and improve research skills in this area. | [SK2] Assessment of progress of work<br>[SK5] Assessment of ability to solve problems that arise in practice |
| [K7_W04] has a structured knowledge of the application of informatics tools in biotechnology and molecular modeling of biomolecules | The student has knowledge of molecular modeling methods such as dynamics and molecular mechanics. | [SW3] Assessment of knowledge contained in written work and projects<br>[SW1] Assessment of factual knowledge |
| [K7_U06] is able to apply statistical methods, computer solutions, especially bioinformatics methods to design experiments and technologies, analyze experimental results and technological processes and solve and technological processes and solve problems in the field of biotechnology, is able to use biotechnological databases | The student knows how to use molecular modeling methods such as molecular dynamics to learn about the molecular properties of biomolecules. | [SU4] Assessment of ability to use methods and tools<br>[SU3] Assessment of ability to use knowledge gained from the subject<br>[SU1] Assessment of task fulfilment |

| | |
|---|---|
| Subject contents | • - Introduction and definition what it is a molecular dynamics and its historical background.<br>• - Definition and characteristics of static and dynamics molecular properties of biomolecules (biopolymers and small organic molecules).<br>• - Definition and characteristics of inter- and intra-molecular interactions.<br>• - Areas and limitations of application of molecular modeling with regard to advancement of different methods.<br>• - Force-fields definition and examples.<br>• - Molecular mechanics and dynamice.<br>• - Overview of molecular mechanics and dynamics software.<br>• - Electrostatic interactions and solvation models applied in molecular modeling.<br>• - Examples of application of molecular dynamics (biopolymers).<br>• - Examples of application of molecular dynamics in simulations of model biological membranes.<br>• - Free energy calculations.<br>• - Molecular docking.<br>• - Modeling of interactions between ligands and molecular targets.<br>• - Computer-aided drug design as well as design other small molecules exhibited required molecular properties.<br>• - AI methods in drug design |
| Prerequisites and co-requisites | Students have to complete previously courses: physical chemistry, mathematics, biochemsitry and biophysics. |

Assessment methods and criteria

| Subject passing criteria | Passing threshold | Percentage of the final grade |
|---|---|---|
| laboratory - practical test | 60.0% | 30.0% |
| test - lecture | 60.0% | 70.0% |

Recommended reading

| | |
|---|---|
| Basic literature | 1. **CH.I. Brookes III, M. Karplus. B.M. Pettitt, Proteins, a theoretical perspective of dynamice, structure, and thermodynamics, Advances in Chemical Physics Volume LXXI, John Wiley & Sons, New York 1988**<br>2. **D.W. Heermann, Podstawy symulacji komputerowych w fizyce, WNT, Warszawa 1997**<br>3. **Ch. J. Cramer, Essentials of Computational Chemistry, theories and models, John Wiley & Sons, New York, 2002**<br>4. **D. Frenkel, B. Smit, Understanding molecular simulation, from algorithms to applications, Academic press, San Diego 2002**<br>5. **T. Schlick, Interdisciplinary Applied Mathematics, Vol. 21, Molecular Modeling and Simulation: An Interdisciplinary Guide, Springer, 2010 (e-book).**<br>6. **J. Czub, Molekularne aspekty aktywności biologicznej amfoterycyny B i jej pochodnych o podwyższonej selektywności badania z zastosowaniem metod chemii obliczeniowej. Praca doktorska, PG 2008.**<br>7. Simone Brogi, Teodorico Castro Ramalho, José L. Medina-Franco, Kamil Kuca and Marian ValkoIn silico methods in drug design and discovery. Frontiers in Chemistry, 2020 (DOI: 10.3389/978-2-88966-057-5).<br>8. Marco Tutone and Anna Maria Almerico, Computational Approaches Drug Discovery and Design in Medicinal Chemistry and Bioinformatics, MDPI 2021 (ISBN: 978-3-0365-2779-6; 978-3-0365-2778-9).<br>9. Rebecca C. Wade and Outi M. H. Salo-Ahen, Molecular Modeling in Drug Design, MDPI 2019 (ISBN: 978-3-03897-615-8)<br>10. Jerzy Leszczynski, Handbook of Computational Chemistry, Springer 2012 (ISBN: 978-94-007-0711-5; 978-94-007-0712-2; 978-94-007-0710-8) 5.Giovanni Ciccotti, Mauro Ferrario and Christof Schuette, Molecular Dynamics Simulation, MDPI 2014 (ISBN: 978-3-906980-65-2; 978-3-906980-66-9). 6.Gerhard Klebe, Drug design, Springer 2013 (DOI 10.1007/978-3-642-17907-5). |
| Supplementary literature | List of scientific papers prepared by the academic teacher given at particular lecture. |
| eResources addresses | Adresy na platformie eNauczanie: |

| | |
|---|---|
| Example issues/ example questions/ tasks being completed | molecular dynamics<br>molecular mechanics<br>drug design<br>molecular docking<br>hydratation in molecular modeling |
| Work placement | Not applicable |

Document generated electronically. Does not require a seal or signature.