GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

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|---|---|---|---|
| Subject name and code | Designing new drugs, PG_00066142 | | |
| Field of study | Chemistry | | |
| Date of commencement of studies | February 2026 | Academic year of realisation of subject | 2026/2027 |
| Education level | second-cycle studies | Subject group | Specialty 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 | 4.0 |
| Learning profile | general academic profile | Assessment form | assessment |
| Conducting unit | Department of Pharmaceutical Technology and Biochemistry -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | dr hab. inż. Tomasz Laskowski | |
| | Teachers | | |

**Lesson types**

| Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
|---|---|---|---|---|---|---|
| Number of study hours | 20.0 | 0.0 | 15.0 | 30.0 | 0.0 | 65 |

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 | 65 | 5.0 | 30.0 | 100 |

**Subject objectives**

The aim of this course is to acquaint students with modern methods of designing chemical molecules with desired properties and especially with desired biological activity. Students will also learn about the mechanisms of drug action at the molecular level, the basic mechanisms of selective toxicity related to it and methods of its determination.

**Learning outcomes**

| Course outcome | Subject outcome | Method of verification |
|---|---|---|
| [K7_U01] integrates and interprets information from literature, databases and other sources | The student is able to find information on the chemistry of natural compounds in databases, understands the structure-activity relationship for biologically active compounds and is able to pre-design new molecules with desired properties using computational methods. | [SU4] Assessment of ability to use methods and tools<br>[SU3] Assessment of ability to use knowledge gained from the subject |
| [K7_W05] defines the principles of sustainable development, national and European conditions for environmental management, in the field of intellectual property protection and patent law | The student understands the complexity of drug design, the time and financial costs associated with this process, and is able to assess the feasibility (or lack thereof) of introducing a new drug for a given disease. | [SW1] Assessment of factual knowledge<br>[SW3] Assessment of knowledge contained in written work and projects |
| [K7_W04] indicates methods for the synthesis of chemical compounds with defined properties | The student possesses the knowledge necessary to construct meaningful and appropriate QSAR and QSPR models based on various approaches to describing the structure of chemical compounds. | [SW1] Assessment of factual knowledge<br>[SW3] Assessment of knowledge contained in written work and projects |
| [K7_K04] is aware of the responsibility for decisions made, observing and developing the principles of professional ethics and working to ensure compliance with these principles | The student understands that falsifying any research results carries enormous risks and entails an inalienable moral responsibility. | [SK5] Assessment of ability to solve problems that arise in practice<br>[SK4] Assessment of communication skills, including language correctness |

<table>
<tr><td>Subject contents</td><td>Course content – lecture<br>• Chemotherapy and selective toxicity<br>• Testing potential chemotherapeutics<br>• Structure-activity relationships<br>• Quantitative structure-activity relationships (QSAR)<br>Course content – laboratory<br>• Optimal dose determination<br>• QSAR + QSPR<br>• Statistical analysis of biological studies<br>Course content – project<br>• Selection of a molecular target<br>• Docking of a ligand library to the selected target<br>• Quantum-chemical characterization of selected ligands<br>• Development of QSAR and QSPR models based on the generated data<br>• Assessment and validation of the resulting models</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>Proficiency in working with spreadsheet software and basic knowledge of the Python programming language.</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>Laboratory reports</td><td>60.0%</td><td>40.0%</td></tr>
<tr><td>Test</td><td>60.0%</td><td>30.0%</td></tr>
<tr><td>Project presentation</td><td>60.0%</td><td>30.0%</td></tr>
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<tr><td>Recommended reading</td><td><table>
<tr><td>Basic literature</td><td>Teaching materials provided by the lecturer</td></tr>
<tr><td>Supplementary literature</td><td>• J. Mazerski, Podstawy chemometrii, Wydawnictwo Politechniki Gdańskiej, Gdańsk, 2000<br>• R. B. Silverman, Chemia organiczna w projektowaniu leków, WNT, Warszawa, 2004</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
</table></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td>• Identify relationships between the antimicrobial activity of a given class of compounds and their physicochemical properties.<br>• Identify relationships between the antimicrobial activity of a given class of compounds and their chemical structure.<br>• Determine the optimal dosage regimen of a given formulation for a specified mouse strain.</td></tr>
<tr><td>Practical activites within the subject</td><td>Not applicable</td></tr>
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