KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI
Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego
UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

| Course title | ECTS code |
|---|---|
| Computationally Added Drug Design | 13.3.1319 |

**Name of unit administrating study**

null

**Studies**

| faculty | field of study | | |
|---|---|---|---|
| Faculty of Chemistry | Chemistry | type | second tier studies (MA) |
| | | form | full-time |
| | | specialty | all |
| | | specialization | all |

**Teaching staff**

prof. dr hab. Tomasz Puzyn; dr inż. Karolina Jagiełło

**Forms of classes, the realization and number of hours**

**Forms of classes**

Laboratory classes

**The realization of activities**

classroom instruction

**Number of hours**

Laboratory classes: 30 hours

**ECTS credits**

2
laboratory classes – 30 h
student's own work – 10 h
tutorial classes – 10 h
Total: 50 h – 2 ECTS

**The academic cycle**

2023/2024 summer semester

**Type of course**

an elective course

**Language of instruction**

english

**Teaching methods**

• Case studies in computer laboratory

**Form and method of assessment and basic criteria for eveluation or examination requirements**

**Final evaluation**

Graded credit

**Assessment methods**

- completion of the final project (written report) related to the design strategy for an imaginary drug,
- observation, how the students discuss the case studies.

**The basic criteria for evaluation**

- completion of the final project (written report) related to the design strategy for an imaginary drug,
- observation, how the students discuss the case studies.

**Method of verifying required learning outcomes**

Written report (K_W01, K_W05, K_W06, K_U01, K_U03).
Discussion of case studies with students (K_W05, K_W06, K_U01, K_U03).
The student identifies the level of their knowledge and skills as well as the need for updating knowledge, continuous professional training, and personal development. (K_K03, K_K04, K_K06).

**Required courses and introductory requirements**

**A. Formal requirements**

None

**B. Prerequisites**

None

**Aims of education**

Developing skills in planning the strategies of computationally added drug design

## Course 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.

## Bibliography of literature

Literature required to pass the course
T. Puzyn, J. Leszczynski (Eds): Towards Efficient Designing of Safe Nanomaterials, RSC Publishing, Cambridge 2012.
A. Gajewicz, T. Puzyn (Eds): Computational Nanotoxicology: Challenges and Perspectives, Jenny Stanford Publishin, 2020.
Extracurricular readings
Research articles published in the following journals:
ACS Nano
Nature Nanotechnology
Nanoscale
Small
Nanotoxicology
Nanomedicine: Nanotechnology, Biology and Medicine
Journal of Nanotoxicology and Nanomedicine

## The learning outcomes (for the field of study and specialization)

K_W01: uses in-depth knowledge of spectroscopic methods of chemical compound analysis

K_W05: has extended knowledge in the field of the specialization studied

K_W06: applies mathematics to the extent necessary to understand, describe and model chemical processes of extended complexity

K_U01: plans and implements chemical experiments of extended complexity

K_U03: finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry

K_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

K_K04: correctly identifies and resolves dilemmas related to the profession of a chemist

K_K06: undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it

## Knowledge

The student knows the possibilities and limitations of computational methods utilized in drug design.

## Skills

The student:
provides examples of computational methods used in drug design,
proposed (selects) appropriate computational drug design strategies.

## Social competence

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

## Contact

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