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		
Wydział Chemii	Chemia	type	drugiego stopnia
		form	stacjonarne
		specialty	Digital Chemistry
		specialization	wszystkie

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

2024/2025 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

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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