KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	ECTS code
QSAR in toxicology	13.3.1312

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

dr Agnieszka Gajewicz-Skrętna; dr inż. Karolina Jagiełło; prof. dr hab. Tomasz Puzyn; mgr Alicja Mikołajczyk

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 winter semester

Type of course

an elective course

Language of instruction

english

Teaching methods

•In the computational laboratory students will conduct hands on exercises
•project-based method (research, implementation, practical project)

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

Final evaluation

Graded credit

Assessment methods

- completion of the final project (building, programming, and testing of a QSAR model for predicting toxicity)
- completion of all assigned projects during classes in the computer lab
- written report for each assigned project

The basic criteria for evaluation

Assessment criteria in accordance with the University of Gdańsk Study Regulations
- correctness of the reports on assigned projects, the final grade of the lab. is based on the partial grades received from each report and presentation of the final project; failure to complete the experimental part means failing the laboratory exercises

Method of verifying required learning outcomes

Written test (K_W03, K_W04, K_W11).
Discussion with the students (K_U05, K_U06).
Observation of the student's behavior during classes and during consultations. (K_K03, K_K07).

Required courses and introductory requirements

A. Formal requirements

lack

B. Prerequisites

Introduction to digital chemistry, introduction to mathematics, introduction to chemistry, introduction to Python/R

Aims of education

Achieving advanced skills in QSAR model development and validation
Familiarizing the students with the available software allowing to develop and validate QSAR model for predicting toxicity
Familiarizing the students with Python/R scripts used in QSAR model development and validation

Course contents

Introduction to collection and curation of data used for QSAR model development
Advanced methods of describing the structural properties of chemicals, methods to select the set of key properties influencing the toxicity, advanced method to define relationships between toxicity and the structural properties including qualitative and quantitative approaches.
Advanced methods of QSAR model validation and applicability domain evaluation.
Methods to report QSAR models, e.g. QMRF.
Review of available software enabling QSAR modeling.

Bibliography of literature

Literature required to pass the course

• R. Kramer: Chemometric techniques for quantitative analysis. New York: Marcel Dekker, Inc, 200
• K. Roy, S. Kar, R. Das Narayan: A Primer on QSAR/QSPR Modeling - Fundamental Concepts. Springer 2015. ISBN: 978-3-319-17281-1.
• T. Puzyn, J. Leszczynski, M. T. D. Cronin: Recent Advances in QSAR Studies: Methods and Applications. Springer 2010. ISBN: 978-1-4020-9782-9.

B. Extracurricular readings

• S. D. Brown, R. Tauler, B. Walczak (red): Comprehensive chemometrics: Chemical and biochemical data analysis. Amsterdam: Elsevier, 2009
• T. Puzyn, A. Mostrąg-Szlichtyng, N. Suzuki, M. Haranczyk. Metody chemometryczne w ocenie ryzyka: Ilościowe za-leżności pomiędzy strukturą chemiczną a właściwościami (QSPR) dla nowych rodzajów zanieczyszczeń chemicznych. W: Zuba D., Parczewski A. (Eds.): Chemometria w nauce i praktyce. Wydawnictwo Instytutu Ekspertyz Sądowych, Kraków (2009). ISBN: 978-83-87425-38-8

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

K_W03: demonstrates in-depth knowledge in the field of modern measuring techniques used in chemical analysis

K_W04: applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis

K_W11: demonstrates in-depth knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field

K_U05: presents the results of research in the form of an independently written paper containing a description and justification of the purpose of the work, adopted methodology, results and their significance in comparison to other similar research

K_U06: presents the results of scientific discoveries in chemistry and related disciplines in an understandable way

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_K07: can think and act in an entrepreneurial manner

Knowledge

At the end of the course every student:
Knows advanced methods applied for QSAR model development and validation
knows basic software packages to be used for QSAR models development and validation
explains theoretical background (algorithm) of the advanced methods for defining the relationships between the structural properties and toxicity

Skills

At the end of the course every student:
uses Python/R environment for developing and validating QSAR model
correctly predicts toxicity by using QSAR model
correctly interprets the results of prediction and is aware of the limitations of QSAR models

Social competence

At the end of the course every student:
is convinced that the use of a QSAR models strengthens the potential of limiting the number of animal tests
can critically evaluate experimental results and understand the necessity of their control
understands the need of deeper learning in computational data analysis and developing predictive models

Contact

agnieszka.gajewicz@ug.edu.pl