University of Gdańsk

Subject card

Subject name and code	QSAR in toxicology, PG_00051256						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject	2027/2028			
Education level	Master's studies		Subject group	Optional subject group			
Mode of study	full-time studies		Mode of delivery	at the university			
Year of study	2		Language of instruction	English			
Semester of study	3		ECTS credits	2.0			
Learning profile	academic		Assessment form	credit			
Conducting unit	Laboratory of Environmental Chemoinformatics -> Department of Environmental Chemistry and Radiochemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Tomasz Puzyn					
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	30.0	0.0	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		5.0	15.0	50	
Subject objectives	• 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						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_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.	Research Presentation: Present research findings in a well-structured, self-edited written paper. Purpose Justification: Clearly describe and justify the purpose of the research. Methodology Explanation: Explain the adopted methodology comprehensively. Result Interpretation: Interpret and present the research results effectively. Relevance Assessment: Assess and discuss the relevance of the results in the context of other similar studies.	[SU2] presentation/project/paper/ report
	[CHEMMU2_W03] Demonstrates extended knowledge in the field of modern measuring techniques used in chemical analysis.	Master QSAR Principles: Understand and apply QSAR models in toxicology. Measurement Techniques: Utilize modern techniques like spectroscopy, chromatography, and mass spectrometry. Data Analysis: Analyze chemical data for toxicological assessments. Critical Evaluation: Evaluate the strengths and limitations of measurement methods. Regulatory Awareness: Understand ethical and regulatory aspects of chemical analysis. Research and Communication: Engage in research and effectively communicate findings.	[SW2] presentation/project/paper/ report
	[CHEMMU2_U06] Presents the results of scientific discoveries in chemistry and related disciplines in an understandable way.	Accessible Presentation: Present scientific discoveries in chemistry and related disciplines in an accessible and understandable manner. Effective Communication: Communicate complex scientific concepts clearly to diverse audiences. Interdisciplinary Understanding: Demonstrate an understanding of interdisciplinary connections between chemistry and related fields. Simplification Skills: Simplify and explain research findings without compromising accuracy. Engaging Delivery: Deliver engaging and informative presentations on scientific discoveries.	[SU2] presentation/project/paper/ report
	[CHEMMU2_W04] Applies the acquired knowledge to an in-depth description of the properties of chemical connections, methods of their synthesis and analysis.	In-depth Chemical Description: Apply QSAR knowledge to describe the properties of chemical combinations comprehensively. Practical Application: Implement acquired knowledge in practical scenarios to analyze chemical properties and predict toxicological effects. Problem-Solving Skills: Develop problem-solving skills to address challenges in the synthesis and analysis of chemical combinations using QSAR models.	[SW2] presentation/project/paper/ report

Course outcome	Subject outcome	Method of verification
[CHEMMU2_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.	Systematic Approach: Demonstrate the ability to work systematically on long-term toxicological projects using QSAR methodologies. Project Management: Understand and apply effective project management techniques to prioritize and complete complex tasks in QSAR research. Prioritization Skills: Develop skills to set and manage priorities to ensure timely completion of multiple tasks in toxicological studies. Strategic Planning: Exhibit strategic planning abilities to manage long-term projects, ensuring alignment with research goals and timelines. Task Execution: Implement efficient task execution strategies to handle various stages of QSAR projects from inception to completion.	[SK2] presentation/project/paper/ report
[CHEMMU2_W11] Demonstrates general knowledge about the current trends in the development of chemistry as a science and the latest discoveries in this field.	Current Developments: Demonstrate comprehensive knowledge of recent advancements in chemistry. Latest Discoveries: Understand and explain the latest discoveries in the field of chemistry. Scientific Awareness: Stay informed about cutting-edge research and trends in chemical science. Integration of Knowledge: Integrate current developments and discoveries into QSAR research and applications. Critical Analysis: Critically analyze new findings and their implications for toxicology and QSAR models.	[SW2] presentation/project/paper/ report
[CHEMMU2_K07] Can think and act in an entrepreneurial manner.	Entrepreneurial Thinking: Develop creative and innovative thinking in QSAR research. Opportunity Exploitation: Identify and act on opportunities in toxicology. Strategic Project Management: Plan and manage QSAR projects entrepreneurially. Problem-Solving: Apply entrepreneurial approaches to solve complex problems. Efficient Resource Use: Manage resources effectively to achieve goals.	[SK2] presentation/project/paper/ report

Subject contents

1. Introduction to collection and curation of data used for QSAR model development

2. 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.

3. Advanced methods of QSAR model validation and applicability domain evaluation.

4. Methods to report QSAR models, e.g. QMRF.

5. Review of available software enabling QSAR modeling.

<table>
<tr><td>Prerequisites and co-requisites</td><td colspan="3">Formal requirements lack

Introductory requirements: Introduction to digital chemistry, introduction to mathematics, introduction to chemistry, introduction to Python/R</td></tr>
<tr><td>Assessment methods and criteria</td><td colspan="3"><table><tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr><tr><td>correctness of the reports on assigned projects</td><td>51.0%</td><td>50.0%</td></tr><tr><td>Final project</td><td>51.0%</td><td>50.0%</td></tr></table></td></tr>
<tr><td rowspan="3">Recommended reading</td><td>Basic literature</td><td colspan="2">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.</td></tr>
<tr><td>Supplementary literature</td><td colspan="2">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</td></tr>
<tr><td>eResources addresses</td><td colspan="2"></td></tr>
<tr><td>Example issues/ example questions/ tasks being completed</td><td colspan="3"></td></tr>
<tr><td>Work placement</td><td colspan="3">Not applicable</td></tr>
</table>

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