University of Gdańsk

Subject card

Subject name and code	Specialization lecture: Molecular descriptors, PG_00117809		
Field of study	Chemistry		
Date of commencement of studies	October 2025	Academic year of realisation of subject	2025/2026
Education level	Master's studies	Subject group	Obligatory subject group in the field of study Optional subject group
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	English
Semester of study	2	ECTS credits	3.0
Learning profile	academic	Assessment form	credit
Conducting unit	Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	dr Alicja Mikołajczyk	
	Teachers	dr Alicja Mikołajczyk dr hab. Celina Sikorska	

Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	0.0	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	40.0	75

Subject objectives	The student knows the possibilities and limitations of molecular descriptors utilized in chemoinformatics, understands the ways of calculating the most important molecular descriptors.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	The student develops the skills of accurate and logical thinking and inference.	[SW4] test/exam - oral or written
[CHEMMU2_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.	The student develops the skills of accurate and logical thinking and inference.	[SK1] oral statement/conversation/ discussion
[CHEMMU2_U01] Plans and implements chemical experiments of medium complexity.	The student develops the skills of accurate and logical thinking and inference.	[SU1] oral statement/conversation/ discussion
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	The student: provides examples of molecular descriptors used for different modelling purposes, proposed (selects) appropriate group(s) of molecular descriptors to be used for solving the problem.	[SW4] test/exam - oral or written
[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	The student: knows the possibilities and limitations of molecular descriptors utilized in chemoinformatics, understands the ways of calculating the most important molecular descriptors.	[SU1] oral statement/conversation/ discussion
[CHEMMU2_U03] Finds necessary information in specialist literature, databases and other sources, lists basic scientific journals in chemistry.	The student develops the skills of accurate and logical thinking and inference.	[SU5] implementation of a problem task
[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	The student develops the skills of accurate and logical thinking and inference.	[SK1] oral statement/conversation/ discussion

Subject contents

Idea of molecular descriptors. Theoretical vs. experimental descriptors. Molecular representation. Classification of molecular descriptors: 1D, 2D, 3D, and 4D descriptors. Topological indexes: molecular graphs, graph-theoretical matrixes, connectivity indexes, characteristic polynomial, spectral indexes. Autocorrelation descriptors: Moreau-Broto autocorrelation descriptors, Moran and Geary coefficients, auto-cross-covariance transforms, autocorrelation of molecular surface properties, atom pairs, Estrada Generalized Topological Index. Geometrical descriptors: indexes from the geometry matrix, WHIM descriptors, GETAWY descriptors, molecular tranforms.

Prerequisites and co-requisites

Math (including Calculus), Quantum Chemistry

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
a multiple-choice question test	51.0%	100.0%

Recommended reading

Basic literature	Literature required to pass the course T. Puzyn, J. Leszczynski, M. T. D. Cronin (Eds): Recent Advances in QSAR Studies: Methods and Applications, Springer, Dodrecht Heidelberg London New York 2010. Extracurricular readings Journal of Chemiformatics Journal of Chemical Information and Modeling SAR and QSAR in Environmental Research
Supplementary literature	Scientific papers in the scope
eResources addresses	

Example issues/ example questions/ tasks being completed

Idea of molecular descriptors. Theoretical vs. experimental descriptors. Molecular representation. Classification of molecular descriptors: 1D, 2D, 3D, and 4D descriptors. Topological indexes: molecular graphs, graph-theoretical matrixes, connectivity indexes, characteristic polynomial, spectral indexes. Autocorrelation descriptors: Moreau-Broto autocorrelation descriptors, Moran and Geary coefficients, auto-cross-covariance transforms, autocorrelation of molecular surface properties, atom pairs, Estrada Generalized Topological Index. Geometrical descriptors: indexes from the geometry matrix, WHIM descriptors, GETAWY descriptors, molecular tranforms.

Work placement

Not applicable

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