

Subject card

Subject name and code	Specialization lecture: Molecular descriptors, PG_00117809						
Field of study	Chemistry						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2024/2025		
Education level	postgraduate 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					
Conducting unit	Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		dr Alicja Mikołajczyk				
	Teachers						
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_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
	[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_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_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_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_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_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	
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 transforms.		
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 Cheminformatics Journal of Chemical Information and Modeling SAR and QSAR in Environmental Research	
	Supplementary literature	Scientific papers in the scope	
	eResources addresses	Adresy na platformie eNauczanie:	
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 transforms.		
Work placement	Not applicable		

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