Uniwersytet Gdański

KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI FUNDUSZ SPOŁECZNY

Course title	**ECTS code**
Specialization lecture: Molecular descriptors	13.3.1297

Name of unit administrating study

null

Studies

faculty	field of study	type	drugiego stopnia
Wydział Chemii	Chemia	form	stacjonarne
		specialty	Digital Chemistry
		specialization	wszystkie

Teaching staff

prof. dr hab. Tomasz Puzyn; dr Agnieszka Gajewicz-Skrętna

Forms of classes, the realization and number of hours	**ECTS credits**
Forms of classes	3
Lecture	classes – 30 h
The realization of activities	tutorial classes – 20 h
classroom instruction	student's own work – 25 h
Number of hours	TOTAL: 75 h – 3 ECTS
Lecture: 30 hours	

The academic cycle

2023/2024 summer semester

Type of course	**Language of instruction**
obligatory	English

Teaching methods	**Form and method of assessment and basic criteria for eveluation or examination requirements**
- discussion	**Final evaluation**
- multimedia-based lecture	Graded credit
	Assessment methods
	Lecture – final test with multiple-choice questions
	The basic criteria for evaluation
	according to "Rules and regulations for studies at the University of Gdansk"
	Lectures: passing the final test in the form of a multiple-choice question test (a score of 50% or more required to pass the exam).

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements

Math (including Calculus), Quantum Chemistry

B. Prerequisites

None

Aims of education

Understanding of the ways of expressing molecular structure by means of molecular descriptors.

Course 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.

Bibliography of 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

The learning outcomes (for the field of study and specialization)	Knowledge
K_W05: has extended knowledge in the field of the specialisation studied	The student: knows the possibilities and limitations of molecular descriptors utilized in chemoinformatics, understands the ways of calculating the most important molecular descriptors.
K_W06: applies mathematics to the extent necessary to understand, describe and model chemical processes of extended complexity	**Skills**
K_U01: plans and implements chemical experiments of extended complexity	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.
K_U02: critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors	**Social competence**
K_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.
K_K01: knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so	
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	

Contact

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