


**KAPITAŁ LUDZKI**  
 NARODOWA STRATEGIA SPÓJNOŚCI

 Projekt współfinansowany przez  
 Unię Europejską w ramach  
 Europejskiego Funduszu  
 Społecznego

**UNIA EUROPEJSKA**  
 EUROPEJSKI  
 FUNDUSZ SPOŁECZNY


<b>Course title</b>		<b>ECTS code</b>	
Statistical mechanics of biological macromolecules		13.3.1313	
<b>Name of unit administrating study</b>			
null			
<b>Studies</b>			
<b>faculty</b>	<b>field of study</b>	<b>type</b>	drugiego stopnia
Wydział Chemii	Chemia	<b>form</b>	stacjonarne
		<b>specjalty</b>	Digital Chemistry
		<b>specialization</b>	wszystkie
<b>Teaching staff</b>			
prof. dr hab. Józef Liwo			
<b>Forms of classes, the realization and number of hours</b>		<b>ECTS credits</b>	
<b>Forms of classes</b>		2	
Auditorium classes		auditorium classes – 30 h	
<b>The realization of activities</b>		tutorial classes – 5 h	
classroom instruction		student's own work – 15 h	
<b>Number of hours</b>		Total: 50 h – 2 ECTS	
Auditorium classes: 30 hours			
<b>The academic cycle</b>			
2024/2025 winter semester			
<b>Type of course</b>		<b>Language of instruction</b>	
an elective course		English	
<b>Teaching methods</b>		<b>Form and method of assessment and basic criteria for evaluation or examination requirements</b>	
During the auditorium classes students will conduct hands on exercises in the computational laboratory, based on the instructions prepared by the teacher.		<b>Final evaluation</b>	
		Graded credit	
		<b>Assessment methods</b>	
		A set of written tests.	
		<b>The basic criteria for evaluation</b>	
		according to "Rules and regulations for studies at the University of Gdansk"	
<b>Method of verifying required learning outcomes</b>			
<b>Required courses and introductory requirements</b>			
<b>A. Formal requirements</b>			
Statistical mechanics in chemistry			
<b>B. Prerequisites</b>			
None			
<b>Aims of education</b>			
The aim of the course is to familiarize students with the basics of statistical mechanics of biopolymers, with particular emphasis on the conditions and mechanisms their structure formation			
<b>Course contents</b>			
Elements of statistical mechanics: ensembles, ensemble averages, thermodynamic connection.			
Statistical-mechanical models of polymers chains.			
Potentials of mean force.			
Structure formation and self-organization in biopolymers as a phase transition.			
One-dimensional case: helix-coil transition.			
Solvent-mediated interactions in the formation and stabilization of biopolymer structure. Polymers in a good and in a bad solvent.			

Global minimum of a potential and of the free energy and stability of polymer structure. Foldability. Simple lattice models to study foldability. Free-energy landscapes of biological macromolecules and methods for their investigation. Coarse-grained force fields for biopolymer simulations as potentials of mean force	
<b>Bibliography of literature</b> D. McQuarrie, Statistical Mechanics, University Science Books, 2000	
<b>The learning outcomes (for the field of study and specialization)</b>  K_W05: has extended knowledge in the field of the specialisation studied  K_W06: applies mathematics to the extent necessary to understand, describe and model chemical processes of extended complexity.  K_U02: critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors  K_U11: communicates in a foreign language in accordance with the requirements specified for level B2 of the Common European Framework of Reference for Languages and can use specialist terminology  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	<b>Knowledge</b>  The student correctly identifies the ensembles, knows, and understands statistical mechanics laws and their application to structure and dynamics of biological macromolecules.
	<b>Skills</b>  The ability to apply the formalism of statistical mechanics to connect the chemical structure of biomolecules with their physicochemical properties.
	<b>Social competence</b>  The student develops the skills of accurate and logical thinking and inference.
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