COURSE SYLLABUS – DOCTORAL SCHOOL
EDUCATION CYCLE FROM 2025/2026 TO 2028/2029

GENERAL INFORMATION ABOUT THE SUBJECT	
Subject title	**RESEARCH METHODOLOGY**
Name of the unit offering the subject	**Doctoral School of the University of Rzeszów**
Type of subject *(compulsory, optional)*	compulsory
Year/semester	First year/first and second semester
Discipline	Biotechnology
Language	English
Name and surname of the course coordinator	Prof. Maciej Wnuk
Name and surname of the course lecturer	Prof. Maciej Wnuk
Prerequisites	Participants should have competences corresponding to level 7 of the Polish Qualifications Framework, confirming their readiness to conduct advanced scientific work in the field of biotechnology. In terms of knowledge, an in-depth understanding of scientific research methodology is required, including knowledge of laboratory procedures, enzyme kinetics and the theoretical foundations of molecular biology and macromolecule biochemistry. The candidate must demonstrate the ability to independently plan and carry out experiments in accordance with the principles of Good Laboratory Practice (GLP) and occupational health and safety. Advanced training in critical analysis of subject literature, efficient use of specialist databases and proficiency in the use of equipment and software supporting research processes are also required. In the area of social competences, candidates must demonstrate a high scientific work ethic, manifested in reliability, responsibility for the research process and conscious compliance with the principles of intellectual property protection and dissemination of research results. Another important skill is autonomy in solving complex research problems, combined with a willingness to cooperate effectively in an interdisciplinary scientific environment, including active participation in national and international knowledge exchange networks.

COURSE SUMMARY

(synthetic description of the content and objectives of the course; 100-200 words)

The course focuses on the application of advanced *in silico* methods in the structural and functional analysis of m^{5}C RNA methyltransferases, with particular emphasis on the NSUN1–7 and TRDMT1 isoforms. The programme combines the theoretical foundations of molecular biology with the practical use of bioinformatics tools in the *Structure-Based Drug Discovery* (SBDD) process. Participants will learn about the stages of research design: from homology modelling and crystallographic analysis, through the identification of active enzyme pockets, to the virtual screening of targeted antiviral drug libraries.

The aim of the course is to equip researchers with the skills necessary to independently conduct projects in the field of molecular engineering. A key element is the analysis of protein-ligand complex stability using molecular dynamics (MD) and pharmacophore optimisation, which allows for the resolution of isoform selectivity issues.

LEARNING OUTCOMES FOR THE COURSE AND VERIFICATION METHODS

Learning outcome symbol	Expected learning outcomes	Reference to learning outcomes for	Form of teaching (lectures, practical classes, etc.)	Assessment methods (e.g. test, oral examination, written

		level 8 PRK qualifications (symbol)		examination, project, etc.)
Knowledge: No.	***knows and understands, has knowledge***			example:
P8S_WG3	He has in-depth knowledge of the mechanisms of action of the epitranscriptome as a therapeutic target, with particular emphasis on the molecular biology of RNA methyltransferases. He is familiar with the theoretical basis of structure-based drug discovery (SBDD) and understands the limitations of classical methods of receptor and kinase modulation.	**P8S_WG**	seminar	preparation of publications, discussion
P8S_WG4	**Possesses knowledge of computational methodology (*in silico*):** Understands the theoretical basis of homology modelling and advanced **molecular dynamics (MD)** simulations. Knows the physicochemical parameters determining the plasticity of protein active sites and the principles of interpreting simulation results in the context of protein-ligand interactions.	**P8S_WG**	seminar	written assignments, discussion
P8S_WK3	Has knowledge of the use of **drug repositioning** strategies through virtual screening of targeted chemical libraries, which enables the effective transfer of basic research results to the therapeutic solutions phase, shortening the process of developing innovative drugs.	**P8S_WK**	seminar	written assignments, discussion
Skills: No.	***is able to***			
P8S_UW1	Is able to integrate advanced computational methods (in silico) into the research process, including the creation of homologous models and conducting advanced molecular dynamics (MD) simulations to analyse the plasticity of protein active sites. Skillfully applies **drug repositioning** strategies through virtual screening of targeted chemical libraries, which allows for the optimization of the translational path of basic research towards therapeutic solutions. Can analyze mechanistic interactions between the inhibitor- nd the SAM substrate, leading to effective pharmacophore optimization.	**P8S_UW**	seminar	written assignments, discussion
P8S_UK1	Able to effectively **confer and present research results** on the epitranscriptomic ecosystem and innovative *in silico* methods, adapting the message to audiences from scientific	**P8S_UK**	seminar	written papers, presentation of research results

	circles and the pharmaceutical industry. Shares the results of their work, participating in discussions on new directions in medical biotechnology.			
P8S_UO1	He is able to actively integrate the results of advanced **molecular dynamics (MD)** simulations and mechanistic analyses with economic needs, thereby promoting the development of modern molecular engineering as a tool with high application value in the global scientific community.	**P8S_UO**	seminar	written assignments
Social competences: No.	***is ready to***			
P8S_KR1	Is ready to conduct scientific activity in an independent and reliable manner, ensuring the highest ethical standards in molecular research. Conducts work on the epitranscriptome and enzyme inhibitors in accordance with the principles of scientific integrity, which builds the credibility of results in the national and international community.	**P8S_KR**	seminar	discussion

FORMS OF TEACHING ACTIVITIES, NUMBER OF HOURS AND CREDITS1

Semester (no.)	Lecture	Exercises	Lab	Practical.	Other	**Number of ECTS points**
I	**-**	**-**	**-**	**-**	**30**	**3**
II	**-**	**-**	**-**	**-**	**30**	**3**
total:	**-**	**-**	**-**	**-**	**60**	**6**

TEACHING METHODS

- traditional seminar;
- seminar with multimedia presentation;
- project;
- discussion.

SYLLABUS

Semester I:

Module 1: Modelling and structural analysis (Fundamentals)

- **Introduction to epitranscriptomics: The role of m⁵C methyltransferases in gene expression regulation.**
- **Advanced protein modelling: Creation and validation of 3D models for NSUN1–7 isoforms (homology, *ab initio* modelling).**
- **Analysis of crystallographic structures: Working with the PDB database in the context of TRDMT1; techniques for verifying the quality of crystallographic structures (electron density maps, evaluation of geometric parameters).**

Module 2: Characterisation of active sites and substrate pockets

- **Identification of binding pockets: Use of geometric and energy algorithms to map the active pockets of methyltransferases.**
- **Analysis of physicochemical properties: Evaluation of hydrophobicity, electrostatic potential and solvent accessibility of the pocket (using CASTp or FPocket servers).**
- **Understanding substrate interactions: Mechanisms of RNA recognition and SAM cofactor binding within the enzyme.**

Semester II:

Module 3: Virtual Screening and Drug Design (Translation)

- **Targeted virtual screening: Methodology for preparing compound libraries (antiviral drugs/existing databases) and preparing ligands for docking.**
- **Molecular docking: Implementation of docking algorithms to identify "hits".**
- **Validation using molecular dynamics (MD): Analysis of protein-ligand complex stability, conformational fluctuations and binding energetics (MM/GBSA methods).**
- **Pharmacophore design: Definition of key features (hydrogen bond acceptors/donors, hydrophobic groups) necessary for selective inhibition of NSUN/TRDMT1.**

COURSE COMPLETION REQUIREMENTS (ASSESSMENT CRITERIA)

The course is taught in semesters I and II. After semester I, the course ends with a ZO1 grade, and after semester II, it ends with an E2 exam. The course is taught through direct contact between the doctoral student and their supervisor or assistant supervisor.

In order to pass the course after the first semester, students are required to submit a report in the form of a research outline describing the implementation of the task. In order to pass the course after the second semester, students are required to obtain at least 51% of the points from the oral examination.

In order to obtain a positive grade, a conversion factor is applied for the corresponding percentage of points obtained:
- up to 50% - fail (the doctoral student is not making progress in their research, is not expanding their knowledge, is not studying the literature, is not participating in substantive discussions, is not fulfilling their academic obligations);
- 51% - 60% - satisfactory (the doctoral student makes negligible progress in scientific research, expands their knowledge, studies basic literature, the discussion is limited to a narrow range of substantive knowledge, fulfils basic scientific duties);
- 61% - 70% - satisfactory plus (the doctoral student makes progress in scientific research, expands their knowledge, studies basic literature, participates substantively in discussions, fulfils their scientific duties);
- 71% - 80% - good (the doctoral student makes significant progress in scientific research, broadens their knowledge, studies basic and supplementary literature, participates substantively in discussions, fulfils all scientific duties);
- 81% - 90% - good plus (the doctoral student makes significant progress in scientific research, systematically expands their knowledge, studies basic and supplementary literature, participates substantively in discussions, fulfils all scientific duties);
- 91% - 100% - very good (the doctoral student makes significant progress in scientific research, systematically expands their knowledge, studies basic and supplementary literature as well as literature beyond the required scope, participates in discussions in a substantive manner, fulfils all scientific obligations);

TOTAL WORKLOAD OF THE DOCTORAL STUDENT REQUIRED TO ACHIEVE THE DESIRED RESULTS IN HOURS AND ECTS POINTS

Form of activity	Average number of hours to complete the activity
Hours spent in direct contact resulting from the study plan	**2 x 30 hours – 60 hours**
Other activities with the participation of a teacher (participation in consultations, examinations)	**10**
Hours completed independently by the doctoral student (preparation for classes, examination, writing a paper, etc.)	**110 hours**
TOTAL HOURS	**180**
TOTAL NUMBER OF ECTS POINTS*	**6**

LITERATURE	
Basic literature:	• Jain, S. et al. (2020). Structure-Based Drug Discovery: An Overview. In: "Methods in Molecular Biology". • Schlick, T. (2010). Molecular Modelling and Simulation: An Interdisciplinary Guide. Springer. • Leach, A. R. (2001). Molecular Modelling: Principles and Applications. Pearson.
Supplementary literature:	• **Sliwoski, G., Kothiwale, S., Meiler, J., & Lowe, E. W. (2014).** *Computational Methods in Drug Discovery*. Pharmacological Reviews. • **Jumper, J. et al. (2021).** *Highly accurate protein structure prediction with AlphaFold*. Nature. • **Wang, J. et al. (2019).** *Drug repositioning: a promising and powerful strategy for rare disease treatment*. Expert Opinion on Orphan Drugs.

**(1 ECTS POINT CORRESPONDS TO 25–30 HOURS OF TOTAL WORK REQUIRED BY A DOCTORAL STUDENT TO ACHIEVE THE INTENDED LEARNING OUTCOMES)*

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Date and signature of the course instructor

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Approval by the Head of the Unit or authorised person