SYLLABUS

Structural bioinformatics and bio-molecular modelling

University year 2025-2026

1. Information regarding the programme

1.1. Higher education institution	**Babeş-Bolyai University**
1.2. Faculty	**Faculty of Biology and Geology**
1.3. Department	**Department of Molecular Biology and Biotechnology**
1.4. Field of study	**Biology**
1.5. Study cycle	**Master**
1.6. Study programme/Qualification	**Bioinformatics**
1.7. Form of education	**With presence**

2. Information regarding the discipline

2.1. Name of the discipline	**Structural bioinformatics and bio-molecular modelling**					Discipline code	**BME1122**
2.2. Course coordinator				**Cojocaru Vlad, PhD Habil., CS I**			
2.3. Seminar coordinator				**Cojocaru Vlad, PhD Habil., CS I**			
2.4. Year of study	**1**	2.5. Semester	**2**	2.6. Type of evaluation	**E/**	2.7. Discipline regime	**Compulsory**

3. Total estimated time (hours/semester of didactic activities)

3.1. Hours per week	**4**	of which: 3.2 course	**2**	3.3 seminar/laboratory	**2**
3.4. Total hours in the curriculum	**56**	of which: 3.5 course	**28**	3.6 seminar/laborator	**28**
Time allotment for individual study (ID) and self-study activities (SA)					**66 hours**
Learning using manual, course support, bibliography, course notes (SA)					24
Additional documentation (in libraries, on electronic platforms, field documentation)					20
Preparation for seminars/labs, homework, papers, portfolios and essays					14
Tutorship					8
Evaluations					4
Other activities:					-
3.7. Total individual study hours	**70**				
3.8. Total hours per semester	**126**				
3.9. Number of ECTS credits	**5**				

4. Prerequisites (if necessary)

4.1. curriculum	Molecular Biochemistry and Biophysics, Cell and Molecular Biology
4.2. competencies	Average computer skills

5. Conditions (if necessary)

5.1. for the course	Room with projector, Online meeting platform
5.2. for the seminar /lab	Laptop, Attendance of all practical/ seminar classes, activities

6.1. Specific competencies acquired [1]

Professional/essential competencies	• Development of the ability to explain fundamental biological processes (replication, transcription, enzyme catalysis) as a consequence of biomacromolecular interactions in a certain context of cell life; • The ability to use bioinformatics databases, prediction, analysis and visualization tools to gain in-depth understanding of the structure and functions of biomacromolecules.; • Development of the capacity for analysis, synthesis and communication of specialized scientific information
Transversal competencies	• Acquiring the necessary information / complementary to the assimilation of the content of the Proteomics disciplines. Transcriptomics, Metabolomics, Applied genomics in human health, Individual bioinformatics project. • Carrying out a research project with all that it implies from the use of specific concepts, the selection and application of study methods, the interpretation of data, to the communication of results.

6.2. Learning outcomes

Knowledge	The student knows: • Structural characterization of biomolecules and biomolecular complexes • Theoretical description of the main methods used în Structural Bioinformatics (Structual modeling, Molecular Dynamics Simulations, Molecular Docking) • Mechanisms of gene regulation and the link between structure and function of biomolecules

[1] One can choose either competences or learning outcomes, or both. If only one option is chosen, the row related to the other option will be deleted, and the kept one will be numbered 6.

Skills	The student is able to: • Visualize structures of biomolecules and enphasize diverse structural properites • Perform Structural Modeling using a range of available methods • Set up and perform Molecular Dynamics Simulations • Set up and perform Molecular Docking • Navigate în the Linux operating system • Write scripts în different programming languages to visualize and analyze data
Responsibility and autonomy:	The student has the ability to work independently to: • Develop a small scale research project from set up to completion • Write a scientific report about a research project according to a pre-defined journal template • Present a scientific article to colleagues

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	• Description of the relationship between the sequence, structure, dynamics and function of biomacromolecules such as nucleic acids and proteins, as well as their interaction products, using databases and dedicated prediction, analysis and visualization methods.
7.2 Specific objective of the discipline	• Understanding the relationship between the nucleotide sequence and the amino acid sequence, as well as between the sequence, structure and functions of proteins; • Explaining the structural principles underpinning macromolecular functions during biological processes; • Application of bioinformatics tools for aligning sequences in order to discover structural motifs and domains of proteins and their classification; • Use of the main computational strategies for the prediction, modelling, simulation, analysis and visualization of the structures of proteins, nucleic acids and their interaction products.

8. Content

8.1 Course	Teaching methods	Remarks
Introduction to structural bioinformatics: definition, purposes and applications.	• Interactive exposure • Presentation • Explanation • Practical examples • Case-study discussions	
Macromolecular structures: levels of structure organization, experimental methods of structure determination, visualization and modeling of 3D structures based on sequence data.		
The relationship between sequence, structure and function în biomolecules.		

Sequence and structure alignments: databases used in structural bioinformatics, classification of biomolecules and their interactions		
The structural bases of macromolecular dynamics, binding specificity: Molecular Dynamics Simulations and Molecular Docking		
Analysis of structures, their dynamics and interactions		

Bibliography

- Eidhammer I., Jonassen I., Taylor W.R., Protein bioinformatics : an algorithmic approach to sequence and structure analysis. Chichester : John Wiley & Sons, 2004
- Rigden D.J. From Protein Structure to Function with Bioinformatics : Springer; 2017
- Keith J.M., Bioinformatics. Vol. 2: Structure, function, and applications. New York : Humana Press, 2017.. In: Bioinformatics, vol. Vol. 2,
- Gaspari Z., Structural Bioinformatics, Springer, 2020
- Leach, A.R. Molecular modelling: principles and applications. 2nd edition, Pearson education.2001.
- Stryer L., Biochemistry. New York : W. H. Freeman and Company, 1995\
- Schlick T., Molecular modeling and simulation : an interdisciplinary guide. New York, Springer, 2010.
- Xiong J., Essential bioinformatics. New York : Cambridge University Press, 2006
- Ramachandran, K. I., Gopakumar, Deepa., Computational Chemistry and Molecular Modeling : Principles and Applications. Berlin, Springer-Verlag, 2008
- Chatenay, D., Multiple aspects of DNA and RNA : from biophysics to bioinformatics /. Amsterdam ; Elsevier, 2005.. URL: http://www.sciencedirect.com/science/book/9780444520814.

References (1-3, 5, 6, 8, 9, 10) are available in printed format at the libraries of the Faculty of Biology and Geology. References (2, 4, 5, 7) are available upon request from the class tutor. Reference (7) is available in printed format at the library of the Faculty of Chemistry and Chemical Engineering.

8.2 Seminar / laboratory	Teaching methods	Remarks
Data collection, analysis and visualization: exercises.	• Practical project • Interactive exposure • Presentation • Explanation • Discussions • Evaluation • Practical feed-back	
Modeling of three-dimensional structures of biomacromolecules: case studies and exercises		
Comparison of 3D structures		
Modeling and visualization of bio-molecular dynamics		
Docking of biomolecules		
Data validation, integration and comparison		
Evaluation of a short individual project on structural bioinformatics topic		

Bibliography

Resurse electronice, baze de date și instrumente bioinformatice disponibile online.
Uniprot (SwissProt, https://www.uniprot.org/), Protein Data Bank (https://www.rcsb.org/), SCOP data base (https://scop.mrc-lmb.cam.ac.uk/), CATH data base (https://www.cathdb.info/), AlphaFold data base (https://alphafold.ebi.ac.uk/)

Software
SwissModel (https://swissmodel.expasy.org/), Modeller (https://salilab.org/modeller/), Pymol (https://pymol.org), Visual Moleular Dynamics (https://www.ks.uiuc.edu/Research/vmd/), Chimera (https://www.cgl.ucsf.edu/chimera/), AMBER (http://ambermd.org/), NAMD (http://www.ks.uiuc.edu/Research/namd/), Gromacs (https://www.gromacs.org/), HADDOCK (https://wenmr.science.uu.nl/haddock2.4/), AUTODOCK (https://autodock.scripps.edu/), ROSETTA, (https://www.rosettacommons.org/software), AlphaFold (https://www.deepmind.com/research/highlighted-research/alphafold),

9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

- The course promotes the gaining of theoretical knowledge and practical skills required for teamwork in the field of research and development in academic entities, but also in R&D units in private companies;
- The course is present in the curriculum of similar specializations at Romanian and foreign Universities.

10. Evaluation

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Percentage of final grade
10.4 Course	Knowledge of concepts and methods from the topics of the course	Written exam (multiple choice with 0 or more correct answers)	30 %
10.5 Seminar/laboratory	Research Project evaluation	Written report (2 pages) according to a scientific journal template	30 %
	Evaluation of presentation skills	Presentation of a research article related to the course topics	30 %
10.6 Minimum standard of performance			
• Each student should obtain minimum 5 at the written exam and oral colloquium. In order to obtain the minimum grade 5, the student must demonstrate the mastery of the basic concepts described during the course and practicum classes.			

11. Labels ODD (Sustainable Development Goals)[2]

	General label for Sustainable Development							
								

Date:

21.01.2025

Signature of course coordinator

Cojocaru Vlad, PhD Habil., CS I

Signature of seminar coordinator

Cojocaru Vlad, PhD Habil., CS I

Date of approval:
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Signature of the head of department

Assoc. Prof. Beatrice Kelemen, PhD

[2] Keep only the labels that, according to the *Procedure for applying ODD labels in the academic process*, suit the discipline and delete the others, including the general one for *Sustainable Development* – if not applicable. If no label describes the discipline, delete them all and write „*Not applicable*.".