SYLLABUS

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 applied in life sciences**

2. Information regarding the discipline

2.1 Name of the discipline (en) / (ro)			**Structural bioinformatics and bio-molecular modelling** **Bioinformatică structurală și modelare biomoleculară**				
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 Type of discipline	**Compulsory**
2.8. Code of the discipline		**BME1122**					

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/laboratory	**28**

Time allotment:	hours
Learning using manual, course support, bibliography, course notes	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	• Genetics, Molecular Biochemistry and Biophysics, Cell and molecular biology
4.2. competencies	• Average computer skills

5. Conditions (if necessary)

5.1. for the course	• Beamer • Online meeting platform
5.2. for the seminar /lab activities	• Attendance of all practical/ seminar classes, • Computers, specific development environment

6. Specific competencies acquired

Professional 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.

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	
The relationship between sequence, structure and function in nucleic acids and proteins.		
Sequence alignment. Databases used in structural bioinformatics. Protein classification and dedicated databases.		
Macromolecular structures: levels of structure organization, experimental methods of structure determination, visualization and modeling of 3D structures based on sequence data.		
Analysis of 3D structures. Prediction of secondary and tertiary structures and functions of biomacromolecules.		
The structural bases of macromolecular dynamics, binding specificity and enzymatic catalysis.		
Structural bioinformatics in systems biology and clinical applications.		

Bibliography

1. Eidhammer I., Jonassen I., Taylor W.R., Protein bioinformatics : an algorithmic approach to sequence and structure analysis. Chichester : John Wiley & Sons, 2004
2. Keith J.M., Bioinformatics. Vol. 1: Data, sequence analysis, and evolution. New York : Humana Press, 2017.. In: Bioinformatics, vol. Vol. 1
3. Keith J.M., Bioinformatics. Vol. 2: Structure, function, and applications. New York : Humana Press, 2017.. In: Bioinformatics, vol. Vol. 2,
4. Leach, A.R. Molecular modelling: principles and applications. Pearson education.2001.
5. Pevzner P., Bioinformatics for biologists. Cambridge ; New York : Cambridge University Press, 2013
6. Stryer L., Biochemistry. New York : W. H. Freeman and Company, 1995\
7. Schlick T., Molecular modeling and simulation : an interdisciplinary guide. New York, Springer, 2010.
8. Xiong J., Essential bioinformatics. New York : Cambridge University Press, 2006

References (1-3, 5, 6, 8) are available in printed format at the libraries of the Faculty of Biology and Geology. Reference (4) is 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.	• Interactive exposure • Explanation • Conversation • Practical demonstration • Case study	
Modeling of three-dimensional structures of biomacromolecules: case studies and exercises		
Comparison of 3D structures		
Modeling and visualization of molecular dynamics		
Data validation, integration and comparison		
Evaluation of a short individual project on structural bioinformatics topic	• Evaluation	

Bibliography

1. Chatenay, D., Multiple aspects of DNA and RNA : from biophysics to bioinformatics /. Amsterdam ; Elsevier, 2005.. URL: http://www.sciencedirect.com/science/book/9780444520814.
2. Ramachandran, K. I., Gopakumar, Deepa., Computational Chemistry and Molecular Modeling : Principles and Applications. Berlin, Springer-Verlag, 2008
3. Schlick T., Molecular modeling and simulation : an interdisciplinary guide. New York, Springer, 2010
4. Electronic resources, databases and bioinformatics tools available online

References (1-3) are available in electronic or printed formats at the libraries of the `Lucian Blaga` Central University Library, Cluj-Napoca.

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

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.1 Course	Knowledge of concepts and methods from the topics of the course	Written exam (combined test)	50%
10.2 Seminar/lab activities	Evaluation of an individual project on structural bioinformatics topic	Oral colloquium	50%
10.3Minimum performance standards			
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.			

Date	Signature of course coordinator	Signature of seminar coordinator
16.01.2023	**Cojocaru Vlad, PhD Habil., CS I**	**Cojocaru Vlad, PhD Habil., CS I**

Date of approval	Signature of the head of department
20.01.2023	**Assoc. Prof. Beatrice Kelemen**