COURSE DESCRIPTION

Structural bioinformatics and biomolecular modelling

Academic year 2026-2027

1. Programme-related data

1.1. Higher Education Institution	Babeș-Bolyai University
1.2. Faculty	Chemistry and Chemical Engineering
1.3. Department	Chemistry
1.4. Field	Chemistry
1.5. Level of study	Master
1.6. Degree programme / Qualification	Chemical biology in life and medical sciences
1.7. Form of education	Full-time education

2. Course-related data

2.1. Course title	Structural bioinformatics and biomolecular modelling			Course code	CME6106
2.2. Course coordinator	Prof. Dr. Horia Banciu/ CS.I Dr. Vlad Cojocaru				
2.3. Seminar coordinator	Prof. Dr. Horia Banciu/ CS.I Dr. Vlad Cojocaru				
2.4. Year of study	1	2.5. Semester	1	2.6. Type of assessment	Progress check
2.7. Course status	Compulsory			2.8. Course type	Core subject

3. Total estimated time (hours per semester of teaching 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)					**68 hours**
3.5.1. Learning using manual, course support, bibliography, course notes (SA)					15
3.5.2. Additional documentation (in libraries, on electronic platforms, field documentation)					20
3.5.3. Preparation for seminars/labs, homework, papers, portfolios and essays					20
3.5.4. Tutorship					8
3.5.5. Evaluations					5
3.5.6. Other activities:					-
3.7. Total individual study hours	**68**				
3.8. Total hours per semester	**126**				
3.9. Number of ECTS credits	**5**				

4. Prerequisites (where applicable)

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

5. Specific conditions (where applicable)

5.1. for the course	• Video logistic support, MS Teams platform, Teaching board • Students will not use mobile phones during the course
5.2. for the seminar /lab activities	• The deadline for submitting assignment results will be agreed upon between the seminar/laboratory coordinator and the students. Delays will not be accepted unless justified by valid reasons. • In the case of late submission, the grade will be penalized by 0.5 points per

	day of delay.

6.1. Competencies resulting from the completion of the degree programme *(as referred to in the curriculum)*[1]

Professional competencies	
Competency code	**Competency**
PC1	Development of the ability to explain fundamental biological processes (replication, transcription, enzyme catalysis) as a consequence of bio-macromolecular 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 bio-macromolecules.
PC3	Development of the capacity for analysis, synthesis and communication of specialized scientific information.
Transversal competencies	
Competency code	**Competency**
TC2	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.
TC3	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 relevant to the degree programme (as referred to in the curriculum)[2]

Learning outcomes targeted by the subject		
Competency code	**Knowledge and comprehension**	**Specific academic skills**
CP1, CP6	1. Knowledge of advanced bioanalytical techniques for understanding of specific interactions in biological systems.	1. Creative use of knowledge of the bioanalytical techniques for the structural and functional analysis of biomacromolecules.
CP6	1. The student/graduate knows the basic principles of a (bio)process, the stages of technology development, and methods for separating useful products. 2. The student/graduate knows the basic principles of a recombinant DNA technology, genetic engineering and the stages of technology development for the production of proteins	1. The student/graduate proposes technologies for obtaining useful products, including their separation/purification steps. 2. The student/graduate proposes technologies for obtaining useful protein products, including their separation/purification steps.

7. Subject-specific learning outcomes

Knowledge and comprehension
1. Structural characterization of biomolecules and biomolecular complexes.
2. Theoretical description of the main methods used in Structural Bioinformatics (Structural modeling, Molecular Dynamics Simulations, Molecular Docking)
3. Mechanisms of gene regulation and the link between structure and function of biomolecules.

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

Specific academic skills
1. Visualize structures of biomolecules and emphasize diverse structural properties; perform Structural Modelling using a range of available methods; set up and perform Molecular Dynamics Simulations; set up and perform Molecular Docking; navigate in the Linux operating system; write scripts in different programming languages to visualize and analyze data.
2. Develop a small-scale research project from set up to completion.
3. Write a scientific report about a research project according to a pre-defined journal template; present a scientific article to colleagues.

8. Contents

8.1 Course	Teaching methods	Remarks
8.1.1. Introduction to structural bioinformatics: definition, purposes, and applications.	Interactive exposure, presentation, explanation, practical examples, case-study discussions	
8.1.2. Macromolecular structures: levels of structure organization, experimental methods of structure determination, visualization, and modeling of 3D structures based on sequence data.	Interactive exposure, presentation, explanation, practical examples, case-study discussions	
8.1.3. The relationship between sequence, structure and function in biomolecules.	Interactive exposure, presentation, explanation, practical examples, case-study discussions	
8.1.4. Sequence and structure alignments: databases used in structural bioinformatics, classification of biomolecules and their interactions.	Interactive exposure, presentation, explanation, practical examples, case-study discussions	
8.1.5. The structural bases of macromolecular dynamics, binding specificity: Molecular Dynamics Simulations and Molecular Docking.	Interactive exposure, presentation, explanation, practical examples, case-study discussions	
8.1.6. Analysis of structures, their dynamics, and interactions.	Interactive exposure, presentation, explanation, practical examples, case-study discussions	

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. *Rigden D.J. From Protein Structure to Function with Bioinformatics: Springer; 2017*
3. *Keith J.M., Bioinformatics. Vol. 2: Structure, function, and applications. New York: Humana Press, 2017.. In: Bioinformatics, vol. Vol. 2,*
4. *Gaspari Z., Structural Bioinformatics, Springer, 2020*
5. *Leach, A.R. Molecular modelling: principles and applications. 2nd edition, Pearson education, 2001.*
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*
9. *Ramachandran, K. I., Gopakumar, Deepa., Computational Chemistry and Molecular Modeling: Principles and Applications. Berlin, Springer-Verlag, 2008*
10. *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. Laboratory / Seminar	Teaching methods	Remarks
8.2.1. Data collection, analysis, and visualization: exercises.	Practical project, interactive exposure, presentation, explanation, discussions, evaluation, practical feedback	

8.2.2. Modeling of three-dimensional structures of biomacromolecules: case studies and exercises.	Practical project, interactive exposure, presentation, explanation, discussions, evaluation, practical feedback	
8.2.3. Comparison of 3D structures.	Practical project, interactive exposure, presentation, explanation, discussions, evaluation, practical feedback	
8.2.4. Modeling and visualization of bio-molecular dynamics	Practical project, interactive exposure, presentation, explanation, discussions, evaluation, practical feedback	
8.2.5. Docking of biomolecules.	Practical project, interactive exposure, presentation, explanation, discussions, evaluation, practical feedback	
8.2.6. Data validation, integration, and comparison.	Practical project, interactive exposure, presentation, explanation, discussions, evaluation, practical feedback	
8.2.7. Evaluation of a short individual project on a structural bioinformatics topic	Practical project, interactive exposure, presentation, explanation, discussions, evaluation, practical feedback	

Bibliography:

1. *Electronic resources, databases, and bioinformatics tools available 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/)

2. *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. Evaluation

Type of activity	9.1 Evaluation criteria[3]	9.2 Evaluation methods[4]	9.3 Percentage in the final grade
9.4. Course	Knowledge of concepts and methods from the topics of the course.	Written exam (multiple choice with 0 or more correct answers) – Access to the exam is conditional on completing the laboratory test and submitting the corresponding laboratory reports for all practical work. Any attempt at cheating during the exam will result in disqualification from the exam. Exam fraud is punishable by expulsion, in accordance with the ECTS regulations of UBB.	30%

[3] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[4] Both final evaluation methods and ongoing evaluation strategies should be established.

9.5 Seminar	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%
9.6 Minimum standard for passing			
✓ 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.			

10. SDG labels (Sustainable Development Goals)[5]

	○	Sustainable Development Generic Label						
								
○	○	◉	○	○	○	○	○	◉
								No label applies
○	○	○	○	○	○	○	○	○

Date of entry:
22.04.2026

Signature of course coordinator

Prof. Dr. Horia Banciu/ CS.I Dr. Vlad Cojocaru

Signature of seminar coordinator

Prof. Dr. Horia Banciu/ CS.I Dr. Vlad Cojocaru

Date of approval in the department:

24.04.2026

Signature of the head of department
Prof. Dr. Eng. Monica Ioana TOȘA

[5] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the subject, select the last option: *"No label applies."*