SYLLABUS

INTEGRATIVE BIOINFORMATICS

ACADEMIC YEAR 2023-2024

1. Information regarding the programme

1.1 Higher education institution	**Babeş-Bolyai University**
1.2 Faculty	**Faculty of Biology and Geology**
1.3 Department	**Doctoral School of Integrative Biology**
1.4 Field of study	**Biology**
1.5 Study cycle	**Doctorate, 3 years**
1.6 Study programme / Qualification	**PhD in Biology/ Biologist**

2. Information regarding the discipline

2.1 Name of the discipline (en) / (ro)		**Integrative Bioinformatics** **Bioinformatică integrativă**					
2.2 Course coordinator		**Cojocaru Vlad, PhD Habil., CS I** **Banciu Horia Leonard, PhD Habil., Prof.**					
2.3 Seminar coordinator		**Cojocaru Vlad, PhD Habil., CS I** **Banciu Horia Leonard, PhD Habil., Prof.**					
2.4. Year of study	**1**	2.5 Semester	**1**	2.6. Type of evaluation	**E**	2.7 Type of discipline	**O**
2.5. Code of the discipline							

E – exam; O – optional

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

3.1 Hours per week	4	Out of which: 3.2 Lectures	1	3.3 Seminars / Laboratory classes	3
3.4 Total hours in the curriculum	48	Out of which: 3.5 Lectures	12	3.6 Seminars / Laboratory classes	36

Allocation of study time:	hrs
Study supported by textbooks, other course materials, recommended bibliography and personal student notes	60
Additional learning activities in the library, on specialized online platforms and in the field	44
Preparation of seminars / laboratory classes, topics, papers, portfolios and essays	50
Tutoring	46
Examinations	4
Other activities: -	-

3.7 Individual study (total hours)	204
3.8 Total hours per semester	252
3.9 Number of credits	10

4. Prerequisites (if necessary)

4.1. Curriculum	• Genetics, Biochemistry, Biophysics, Cell and molecular biology
4.2. Competencies	• Average computer skills

5. Conditions (if necessary)

5.1. for the course	• Beamer, blackboard; • Internet connection; Online meeting platform
5.2. for the seminar /lab activities	• Attendance of all (100%) practical/ seminar classes, • Computers, specific development environment

6. Specific competencies acquired

Professional competencies	- Ability to use Linux and command line interfaces in life sciences; - Development of the ability to generate, integrate, and analyse sequence data for life sciences; - The ability to use bioinformatics databases, prediction, analysis and visualization tools to model and predict protein structures and protein-nucleic acid complexes; - The ability to use basic methods for molecular dynamics simulations - The ability to use bioinformatics databases, prediction, analysis and visualization tools to infer the diversity and functionality of microbial communities in natural ecosystems; - Development of the capacity for analysis, synthesis and communication of specialized scientific information
Transversal competencies	- Acquiring the necessary information to complete a doctoral thesis in Biology field in which generation, processing and analysis of high-throughput data is central. - Carrying out a research project with all that implies 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	Gaining knowledge on the structure and dynamics of proteins, nucleic acids and other biological macromolecules, as well as diversity and ecological roles of microbial communities using databases and dedicated prediction, analysis and visualization methods.
7.2 Specific objective of the discipline	- Developing the capacity to analyze and interpret structures of biomolecules and to link the structures with biological function; - Developing the skills to follow an inter-disciplinary approach to study biomolecules; - Understanding the principles of generation and processing of high-throughput sequence data by NGS; - Use of the main computational strategies for the prediction, modelling, analysis and visualization of community diversity and its ecological functions. - Developing the skills to summarize and disseminate scientific literature in structural and environmental bioinformatics.

8. Content

8.1 Course	Teaching methods *Hybrid teaching: 40% onsite and 60% online (MS Teams/Zoom) classes*	Remarks
Structural Bioinformatics (part I) Introduction to Linux **Structural Bioinformatics (part II)** Visualization and analysis of biomolecular structures (e.g. proteins, nucleic acids) **Structural Bioinformatics (part III)** Molecular modelling (prediction of biomolecular structures, structure-based design)	- Interactive exposure - Presentation - Explanation - Practical examples - Case-study discussions	6 hours

Structural Bioinformatics (part IV) Molecular docking, molecular dynamics simulations, free energy calculations		
Environmental Bioinformatics (part I) **1. Phylogeny & probe design (ARB-SILVA)** 1.a. Work with 16S rRNA gene sequences. Assemble full-length 16S sequences from multiple sequences. Primer removal. Chimera check. 1.b. Introduction to ARB. Import fasta files to ARB. Generate unique file names. Sequence alignment to SILVA database. Manual inspection and correction of alignment. 1.c. Add aligned seqs to ARB tree. Calculate phylogenetic trees. Bootstrap values. Choice of root sequences. Tree design & export. 1.d. Introduction to probe design tool in ARB. Design oligonucleotide probes. Criteria for probe selection and in silico testing.	- Interactive exposure - Presentation - Explanation - Practical examples - Case-study discussions	6 hours
Environmental Bioinformatics (part II) **2. Community fingerprinting by amplicon sequencing (Illumina reads)** 2.a. Work with raw reads (fastq files). Sequence processing: primer/adapter removal (cutadapt, BBMap, Illumina bcl2fastq). Pairing of processed sequences (BBMerge), quality filtering (USEARCH, QIIME2), removal of chimeras (USEARCH, QIIME2) and dereplication (USEARCH, QIIME2). 2.b. OTU/ASV clustering of processed reads. Work with DADA2 R, SWARM, MetaAmp or QIIME2 pipelines. Taxonomic allocation of OTU/ASVs based on SilvaNGS pipeline. Work with the online SilvaNGS engine. Generate Krona plots.		
Environmental Bioinformatics (part III) **3. Metagenomics** 3.a. Quality control of raw data. Adapter clipping. Merge unpaired reads into a single file. Trimmomatic, BBduk 3.b. Metagenome assembly (Spades). Assembly evaluation (MetaQuast). Extraction of 16S from contigs (rnammer), chimeras detection (uchime). Gene prediction (prodigal). Blast with custom databases for search of specific genes/proteins. 3.c. Binning (MetaBAT or MaxBin). Completeness and contamination of MAGs, establish criteria for selection (CheckM). Read mapping to MAGs to estimate read abundance of the MAGs (Bowtie, BBmap). Gene prediction (prodigal), annotation of predicted genes/enzymes (KEGG, Pfam, COG). 3.d. Using CheckM and BUSCO, and GTDBTK for genome taxonomy, ANI and AAI for genome comparison.		

Bibliography

1. Keith J.M., Bioinformatics. Vol. 1: Data, sequence analysis, and evolution. New York : Humana Press, 2017.. In: Bioinformatics, vol. Vol. 1

2. Keith J.M., Bioinformatics. Vol. 2: Structure, function, and applications. New York : Humana Press, 2017.. In: Bioinformatics, vol. Vol. 2,
3. Leach, A.R. Molecular modelling: principles and applications. Pearson education.2001.
4. Pevzner P., Bioinformatics for biologists. Cambridge ; New York : Cambridge University Press, 2013
5. Stryer L., Biochemistry. New York : W. H. Freeman and Company, 1995\
6. Schlick T., Molecular modeling and simulation : an interdisciplinary guide. New York, Springer, 2010.
7. Xiong J., Essential bioinformatics. New York : Cambridge University Press, 2006
References (1-2, 4-5, 7) are available in printed format at the libraries of the Faculty of Biology and Geology. Reference (3) is available upon request from the class tutor. Reference (6) is available in printed format at the library of the Faculty of Chemistry and Chemical Engineering.

8.2 Seminar / laboratory	Teaching methods *Hybrid teaching: 50% onsite and 50% online (MS Teams/Zoom) classes*	Remarks
Study cases and exercises in structural bioinformatics (Modeling of three-dimensional structures of biomacromolecules; Comparison of 3D structures; Modelling and visualization of molecular dynamics; Data validation, integration and comparison)	Interactive explanations Explanation Conversation Case study	18 hours
Study cases and exercises in phylogeny and probe design, community-level fingerprinting by amplicon sequencing and metagenomics		18 hours
Presentation of a relevant scientific article		
Evaluation of a short individual project on structural or environmental bioinformatics	• Evaluation	
Bibliography Collection of research articles available in digital format at the libraries of the Faculty of Biology and Geology and `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 and research entities, but also in R&D units in private companies;
- The course is present in the curriculum of similar specializations at USA and European Universities.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade/qualification (%)
10.1 Course	Knowledge of concepts and methods from the topics of the course	Written exam (combined test)	40%
10.2 Seminar/lab activities	Evaluation of -presentation of a research article; - individual project on structural bioinformatics topic	Oral colloquium	20% 40%
10.3 Minimum performance standards			

Each student should obtain a minimum qualification of "SUFFICIENT" (from the following list of available qualifications: INSUFFICIENT / SUFFICIENT / GOOD / VERY GOOD) at the written exam and the oral colloquium. In order to obtain the qualification "SUFFICIENT", 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
28.03.2023	**COJOCARUVlad, PhD Habil., CS I**	**COJOCARU Vlad, PhD Habil., CS I**

BANCIU Horia, PhD Habil., Prof.   **BANCIU Horia, PhD Habil., Prof.**

Date of approval   Signature of the head of department
29.03.2023   **Prof. dr. *Habil*. PAP Peter Laszlo**