UAB Universitat Autònoma de Barcelona	<b>Bioinformatics</b> Code: 100948 ECTS Credits: 3		2024/2025
Degree		Туре	Year

OB

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# Contact

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## Teachers

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# **Teaching groups languages**

You can view this information at the <u>end</u> of this document.

## Prerequisites

There are no prerequisites for this subject, but it is necessary to review the concepts acquired in the subjects of "Biochemistry", "Genetics and Molecular Biology" and "Recombinant DNA Technology" taught during the first and second year.

## **Objectives and Contextualisation**

The subject taught during this course is an introductory vision of bioinformatics. This subject is aimed at students of Biotechnology of the third year (5th semester) and corresponds to a theoretical subject of 3 credits. The objectives and contents of this subject have been defined taking into account that within the same subject (Molecular Biology of Systems) is the subject of "Genomics, Proteomics and Interactomics."

The main objectives are:

- To provide students with basic bioinformatic knowledge that allows both the use of tools to search for information in molecular databases and address the computational analysis of sequences and structures of nucleic acids and proteins.
- Provide a broad perspective of the potential of this discipline both in the field of research and in the professional.

# **Learning Outcomes**

- 1. CM25 (Competence) Work collaboratively in teams to solve problems in the field of systems biology.
- 2. KM25 (Knowledge) Describe the physical and chemical bases of the methodology and instrumentation used in genomic, transcriptomic, proteomic, interactomic and metabolomic analysis.
- 3. KM25 (Knowledge) Describe the physical and chemical basis of the methodology and instrumentation used in genomic, transcriptomic, proteomic, interactomic and metabolomic analysis.
- 4. SM25 (Skill) Analyse information from databases and software necessary for the study of correlations between structure, function and evolution of macromolecules.

## Content

Lesson 1- Introduction. Data banks in Molecular Biology. Search engines: Entrez and SRS. Primary and secondary data banks. Search in specialized databases. Identification of proteins by means of searches in databases.

Lesson 2- Analysis of sequential DNA information. Restriction maps (cloning). Design of probes and oligonucleotides for PCR for the detection and quantification of a sequence, cloning or directed mutagenesis. Secondary structure of RNA.

Lesson 3- Genome Projects and Genomic Browsers. Sequencing, ensemble and annotations of genomes. Identification of coding sequences and promoters.

Lesson 4- Sequence alignments. Concepts of homology and similarity. Algorithms of alignment for sequence pairs. Dot-Plot. Global and local alignment. Punctuation array Gaps Search by similarity in databases: BLAST and FASTA.

Lesson 5- Creation and analysis of multiple sequences alignments: multiple sequence alignment. Editing and viewing programs. Evaluation of conserved regions of proteins. Design of probes and oligonucleotides for PCR based on a multiple alignment of protein sequences. Phylogenetic trees.

Lesson 6-Proteins: analysis of function. Identification of homologues, motifs, domains, and protein families. Identification of distant homologues through PSI-Blast. Statistical models that relax the frequency of an amino acid in a specific position (PSSM matrices, profiles, and hidden Markov model HMM). Prediction of motives and domains. Databases of motives, domains, and protein families. Representation of LOGOS of reasons or emprents.

Lesson 7\_ Protein Structure: prediction, classification, and analysis. Methods for predicting the structure of globular proteins: ab initio-based, homology-based, and neural networks. Evaluation of the reliability of prediction methods. Prediction of the structure of membrane proteins with transmembrane helices and beta barrels. Prediction of coiled-coil structures. Methods for predicting tertiary structure. The PDB structure database. Visualization and comparison of structures. Sequence-based predictions, identification of therapeutic targets. Structure-based predictions. Redesign of protein solubility.

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Classes in the computer room	20	0.8	
Theoretical classes	6	0.24	
Type: Supervised			

# Activities and Methodology

Tutorials	5	0.2
Type: Autonomous		
Study	40	1.6

The teaching methodology includes two types of different activities: theory classes and practical classes in the computer classroom.

## Theoretical Classes

Classes to transmit the basic concepts and the information necessary to develop an autonomous learning. Theory classes will be non-contact and will be taught through audiovisual support. Support in the form of presentations in PowerPoint that will be available to the student on the Virtual Campus.

#### Computer classroom practices or Problems

This activity will take place in the computer rooms of the Faculty and will be carried out in groups of 20 students. These practices will be organized based on problems raised by the teachers and that the student will have to solve using the different tools and bioinformatics analysis. The teacher in each session will pose different problems that will be made in each session or they will have to be solved by the students as autonomous work. At the end of each session, students must submit the corresponding problems to each session. This delivery will be made through the virtual campus.

Attendance at problem sessions and delivery of exercises is mandatory.

#### Tutorials

Individual sessions or small groups for the resolution of doubts related to the subject. This type of activity will be done at the request of the students.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

# Assessment

## **Continous Assessment Activities**

Title	Weighting	Hours	ECTS	Learning Outcomes
Problems done in the sessions on the computer room.	30%	0	0	CM25, KM25, SM25
Written test 1	35%	2	0.08	KM25, SM25
Written test 2	35%	2	0.08	KM25, SM25

The competencies of this subject will be assessed through continuous evaluation, which will be based on the following items:

- Written exams
- Submission of problems solved in the computer lab sessions
- Submission of the integrative project

#### a) Written exams:

These will consist of two partial exams (topics 1-4, part 1; topics 5-7, part 2) that will include short questions and/or multiple-choice questions to relate concepts and problem-solving. They will preferably be held in the computer labs of the Faculty, so that the student will have all the necessary bioinformatics tools available to answer the questions, as well as a list of the links worked on.

Each partial exam will account for 35% of the final grade.

The grade obtained in the assessment activities will only be averaged with the grade of the problems if the average of the two partial exams is 5 or higher.

b) Problem-solving in computer lab sessions:

This assessment will consist of the submission, in groups of two, of all the problems solved in the lab. The submission of the assignments can only be done through the Virtual Campus during the period proposed by the professor. Failure to submit the assignments through the Virtual Campus will be penalized with a grade of 0. Additionally, the submission of the integrative project of the subject, which will count for 20%, will be assessed.

The weight of this assessment will be 30% of the final grade.

#### Single assessment:

The single assessment will consist of: a first part where the theoretical-practical contents taught during the course will be evaluated (this part will count for 70%); a second part where problems will be solved or cases worked on during the lab sessions will be discussed (this part will count for 30%).

Make-up exam and grade improvement:

To participate in the make-up exam, students must have previouslybeen assessed in a set of activities whose weight is equivalent to at least two-thirds of the total grade for the subject or module. Therefore, students will receive the grade "Not assessable" when the assessment activities performed have a weighting of less than 67% in the final grade.

The make-up exam will have the same format as the written exams, i.e., multiple-choice questions and problem-solving. It will also be held in the Faculty's computer labs on the scheduled date.

#### Grade improvement:

Students who wish to improve their grade may take a grade improvement exam at the end of the semester, on the date and place scheduled for the make-up exam. The difficulty level of this exam will correspond to its objective and may therefore be higher than the other written exams. Students who take the grade improvement exam will forfeit the previously obtained grade.

The grade obtained in the lab assignments cannot be modified.

Final grade weighting formula:

Final grade = (Assessment 1 \* 0.35) + (Assessment 2 \* 0.35) + (Problems 1 \* 0.15) + (Problems 2 \* 0.15)

#### General considerations on assessment:

To pass the subject, it is necessary to obtain a final grade of 5 or higher. The final grade will be obtained by averaging the three assessment activities. There will be no averaging if a grade of 5 or higher is not obtained in the written exams or the make-up exam. If the grade of the written exams and/or the make-up exam is below 5, the subject cannot be passed.

Students who cannot attend a written exam for a justified reason and provide the corresponding official documentation to the Degree Coordinator will be entitled to take an exam on another date, which may combine problem-solving and oral responses to questions posed by the professor.

The Degree Coordinator will ensure the arrangement of this with the professor of the affected subject.

Any aspect not covered in this guide will follow the assessment regulations of the Faculty of Biosciences.

# Bibliography

Baxevanis, A. D., Bader, G. D., & Wishart, D. S. (2020). Bioinformatics (Fourth edition). Wiley.

Pevsner, J. (2015). Bioinformatics and Functional Genomics. (3rd ed.). John Wiley & Sons.

Bioinformatics: Sequence and Genome Analysis (Fourth Edition) (2021) by David W. Mount

Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins (Fourth Edition) (2017) by Andreas D. Baxevanis, B. F. Francis Ouellette, and Michael J. E. Sternberg

Introduction to Bioinformatics (Fourth Edition) (2018) by Arthur M. Lesk

Bioinformatics Data Skills: Reproducible and Robust Research with Open Source Tools (Second Edition) (2020) by Vince Buffalo

Exploring Bioinformatics: A Project-Based Approach (Third Edition) (2018) by Caroline St. Clair and Jonathan E. Visick

## Software

Program JalView (www.jalview.org). multialignment representation

PyMol

Links of data bases and applications:

NCBI/nucleotide

https://www.ncbi.nlm.nih.gov/nucleotide/

NCBI/Gene

http://www.ncbi.nlm.nih.gov/gene/

Uniprot

http://www.uniprot.org/

BRENDA

http://www.brenda-enzymes.org/

Swiss-2DPAGE

http://us.expasy.org/ch2d/

Proteome SD-PAGE database

http://web.mpiib-berlin.mpg.de/cgi-bin/pdbs/2d-page/extern/index.cgi

# String

http://string-db.org/
OMIM
http://www.omim.org/
Phosphosite
http://www.phosphosite.org/homeAction.do;jsessionid=117096AF4D54A36677C243A7D586DF45
Nebcutter
http://tools.neb.com/NEBcutter2/
Netprimer
http://www.premierbiosoft.com/netprimer/
Primer3plus
http://www.bioinformatics.nl/cgi-bin/primer3plus/primer3plus.cgi
PrimerBlast
http://www.ncbi.nlm.nih.gov/tools/primer-blast/
ClustalW 2
http://www.ebi.ac.uk/Tools/msa/clustalw2/
Jalview
http://www.jalview.org/download
Uniprot
https://www.uniprot.org/
Paquete T-COFFE
http://tcoffee.vital-it.ch/apps/tcoffee/index.html
Predictor NPSA:
http://npsa-pbil.ibcp.fr/cgi-bin/npsa_automat.pl?page=/NPSA/npsa_server.html
Jalview
http://www.jalview.org/download
Prosite:

## http://prosite.expasy.org/

InterProScan 4

http://www.ebi.ac.uk/Tools/pfa/iprscan/

## PRATT

http://web.expasy.org/pratt/ WebLogo http://weblogo.berkeley.edu/logo.cgi JPred3 http://www.compbio.dundee.ac.uk/www-jpred/ Predict Protein https://predictprotein.org/ COILS http://embnet.vital-it.ch/software/COILS\_form.html Phobius http://phobius.sbc.su.se/ Signal Peptide http://www.cbs.dtu.dk/services/SignalP/ PRED TMBB http://bioinformatics.biol.uoa.gr/PRED-TMBB/input.jsp RCSB PDB http://www.rcsb.org/pdb/home/home.do PDBsum http://www.ebi.ac.uk/pdbsum/ VAST https://www.ncbi.nlm.nih.gov/Structure/VAST/vast.shtml Dali http://ekhidna.biocenter.helsinki.fi/dali\_lite/start EXPASY: www.expasy.org Aggrescan: http://bioinf.uab.es/aggrescan/ Aggrescan 3D

http://biocomp.chem.uw.edu.pl/A3D2/

# Language list

Name	Group	Language	Semester	Turn
(PLAB) Practical laboratories	431	Catalan/Spanish	first semester	morning-mixed
(PLAB) Practical laboratories	432	Catalan/Spanish	first semester	morning-mixed
(PLAB) Practical laboratories	433	Spanish	first semester	morning-mixed
(PLAB) Practical laboratories	434	Spanish	first semester	morning-mixed
(TE) Theory	43	Catalan/Spanish	first semester	morning-mixed