

## **Bioinformatics**

Code: 100948 ECTS Credits: 3

Degree	Туре	Year	Semester
2500253 Biotechnology	OB	3	1

# Contact

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## **Teaching groups languages**

You can check it through this <u>link</u>. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

# Teachers

Nathalia Varejao Nogueira

# 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.

# Competences

2023/2024

- Interpret experimental results and identify consistent and inconsistent elements.
- Learn new knowledge and techniques autonomously.
- Make an oral, written and visual presentation of one's work to a professional or non-professional audience in English or in one's own language.
- Obtain information from databases and use the software necessary to establish correlations between the structure, function and evolution of macromolecules.
- Reason in a critical manner
- Search for and manage information from various sources.
- Search for, obtain and interpret information from the principal databases on biology, bibliography and patents and use basic bioinformatic tools.
- Use ICT for communication, information searching, data processing and calculations.
- Work individually and in teams

## **Learning Outcomes**

- 1. Establish structural, functional and evolutionary relations based on information in existing biological databases .
- 2. Interpret experimental results and identify consistent and inconsistent elements.
- 3. Learn new knowledge and techniques autonomously.
- 4. Make an oral, written and visual presentation of one's work to a professional or non-professional audience in English or in one's own language.
- 5. Obtain, interpret and use information from databases on biology, bibliography, patents, markets, etc.
- 6. Reason in a critical manner
- 7. Search for and manage information from various sources.
- 8. Use ICT for communication, information searching, data processing and calculations.
- 9. Work individually and in teams

## 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\_ Proteins: analysis of structure. Prediction methods of globular protein proteins, ab-initio based, based on homology and neural networks. Evaluation of the reliability of the prediction methods. Prediction of

the structure of membrane proteins with transmembrane helix and beta barrel. Prediction of "coiled-coil". Analysis and prediction of the three-dimensional structure: Methods of prediction of the tertiary structure. The bank of PDB structures. Visualization and comparison of structures. Structural classification of proteins.

Lesson 8- Proteins: analysis and prediction of the folding and aggregation of proteins. Sequence-based predictions, identification of therapeutic targets. Predications based on structure. Redesign of protein solubility.

## Methodology

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.

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Classes in the computer room	20	0.8	3, 8, 7, 1, 4, 2, 5, 6, 9
Theoretical classes	6	0.24	3, 8, 7, 1, 5
Type: Supervised			
Tutorials	5	0.2	8, 7, 2, 5, 6
Type: Autonomous			
Study	40	1.6	3, 8, 7, 1, 2, 5, 6, 9

## Activities

# Assessment

The competences of this subject will be evaluated through continuous evaluation. There will be two types of evaluation:

- Written tests
- Submit exercises made in the sessions on the computer room
- Submit the integrative work

### A) Written tests,

It will consist of two written tests, the first will include topics 1-4 (part 1) and the second topics 5-8 (part 2). Each test will consist of short questions and the resolution of problems. They will be made preferably in the computer rooms of the Faculty so that the student will have at his disposal all the bioinformatics tools necessary to answer the questions and problems raised.

The weight of each test will be 30% of the final mark.

In order to calculate the average mark of the subject, it is essential to obtain a minimum grade of 4 out of 10 in both exams. In case of not reaching the minimum mark in one of the two written tests, the student must take a make-up exam.

B) Resolution of problems in the sessions of the computer room.

It is an individual evaluation that will consist of the hand-in all the problems carried out in the laboratory. The hand-in of the practices has to be done through the Virtual Campus in the period proposed by the professor. Failure to submit the exercises through the Virtual Campus will be penalized. Likewise, the integrative work of the subject will be evaluated.

The weight of this evaluation will be 40% of the final mark.

### Unique evaluation

The unique evaluation will consist of a first part where the theoretical-practical contents taught during the course will be assessed (this part will have a weight of 60%); a second part where problems will need to be solved or cases discussed from the classroom practices (this part will have a weight of 40%).

The mark obtained in this evaluation activity can only average the mark of the written tests if the average of the two partial exams is greater than or equal to 5.

### Retake process

To be eligible for the retake process, the student should have been previously evaluated in a set of activities equaling at least two-thirds of the final score of the course or module. Thus, the student will be graded as "No Avaluable" if the weighting ofall conducted evaluation activities is less than 67% of the final score.

The retake exam will have the same format as the written tests, that is multiple choice questions and problem-solving. It will also be held in the computer rooms of the Faculty on the scheduled date.

### Improvement of the final mark

Students who wish to improve their grades may take a note improvement exam at the end of the semester, on the date and place scheduled for the recovery exam. The degree of difficulty of this test will correspond to the objective of the test and, therefore, may be higher than the other written tests. The student who presents himself to improve the grade waives the previously obtained mark in the evaluation of the written test that he recovers.

Marks obtained in practice sessions can not be modified.

### Calculation of final mark

Final note = (Evaluation 1 \* 0.30) + (Evaluation 2 \* 0.30) + (Problems 1 \* 0.20) + (Problems 2 \* 0.20)

### General Considerations on the Evaluation

To pass the subject it is necessary to obtain a final grade equal to or greater than 5. The final grade will be obtained using the weighted average of the three assessment activities. The average will not be done if you do not get a score equal to or greater than 5 in the written or retake tests of each part.

The revision of the written testswill be carried out on a concerted day and place, between 1 and 7 working days after the publication of the notes.

Students who cannot attend a written test for a justified cause and provide the official documentation corresponding to the Degree Coordinator will have the right to perform on another date a test that could combine the resolution of problems and the oral response to questions raised by the teacher.

The degree coordinator will ensure the specification of this with the teacher of the subject affected.

Any aspect that is not contemplated in this guide will follow the regulations of evaluation of the Faculty of Biosciences.

### **Assessment Activities**

Title	Weighting	Hours	ECTS	Learning Outcomes
Problems done in the sessions on the computer room.	40%	0	0	3, 8, 7, 1, 4, 2, 5, 6, 9
Written test 1	30%	2	0.08	3, 8, 7, 1, 2, 5, 6, 9
Written test 2	30%	2	0.08	3, 8, 7, 1, 2, 5, 6, 9

## **Bibliography**

Bioinformatics: Sequence and Genome Analysis (Fourth Edition) by David W. Mount Author: David W. Mount Year: 2021 Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins (Fourth Edition) by Andreas D. Baxevanis, B. F. Francis Ouellette, and Michael J. E. Sternberg Authors: Andreas D. Baxevanis, B. F. Francis Ouellette, and Michael J. E. Sternberg Year: 2017 Bioinformatics and Functional Genomics (Third Edition) by Jonathan Pevsner Author: Jonathan Pevsner Year: 2015 Introduction to Bioinformatics (Fourth Edition) by Arthur M. Lesk Author: Arthur M. Lesk Year: 2018 Bioinformatics Data Skills: Reproducible and Robust Research with Open Source Tools (Second Edition) by Vince Buffalo Author: Vince Buffalo Year: 2020 Exploring Bioinformatics: A Project-Based Approach (Third Edition) by Caroline St. Clair and Jonathan E. Visick Authors: Caroline St. Clair and Jonathan E. Visick Year: 2018

## 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/