

Degree programme	Type	Course
Biochemistry	OB	3

Contact lecturer

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Prerequisites

There are no pre-requisites for this subject.

It is recommended that the student refreshes the core concepts from "Biologia Molecular" and "Química i Enginyeria de Proteïnes" (2nd year).

Objectives

This course provides an introduction to bioinformatics.

Upon completion of the course, the student should be able:

- To understand the relevance of the availability of public and annotated databases in the development of sequence-based predictive tools.
- To master the most important web-based and/or graphical user interface tools for the study of sequences.
- To obtain, align, visualise and compare sequences.
- To infer phylogenetic relationships among sequences.
- To be familiar with the different predictive tools for sequences, and to be able to choose the best suited to each different experimental question.
- To be able to design simple bioinformatics experiments to answer biochemical questions.

Learning outcomes

- CM19 (Appreciate the contribution of systems biology to innovative solutions for societal needs.) Appreciate the contribution of systems biology to innovative solutions for societal needs.
- KM24 (Quantitatively illustrate a biological process or system.) Quantitatively illustrate a biological process or system.
- KM25 (Describe the main methods of analysis and prediction used in systems biology.) Describe the main methods of analysis and prediction used in systems biology.
- SM21 (Use digital resources when searching databases, analysing genomic, transcriptomic and proteomic data, and creating models of biological systems.) Use digital resources when searching databases, analysing genomic, transcriptomic and proteomic data, and creating models of biological

systems.

- SM24 (Interpret experimental information in the field of systems biology.) Interpret experimental information in the field of systems biology.

Contents

- Bioinformatics. Biomedical databases, public, centralised repositories, formats, controlled vocabularies and data standardisation for exchange and reanalysis.
- Alignment of two sequences. PAM and BLOSUM matrices. Alignment algorithms.
- "Basic Local Alignment Search Tool" (BLAST). BLAST search algorithm. Parameters and basic BLAST types. Evaluation of BLAST results.
- PSI-BLAST and other advanced types of BLAST searches. The "position-specific scoring matrix" (PSSM).
- Multiple sequence alignment (MSA). MSA strategies: exact, progressive, iterative, consistency-based or structure-based.
- MSA databases: Pfam and "Conserved domain database".
- Phylogenies. Phylogenetic tree types and components. Steps and methods to build and evaluate a phylogenetic tree.
- Domains. Protein modularity and development of search and/or prediction tools. Bioinformatic tools for predicting the physical properties, location and function of proteins.
- Principles of protein structural prediction. The Chou and Fasman algorithm. Homology-based, fold-recognition or "ab-initio" strategies. Structural visualisation tools. Protein databases (Unoprot, PDB), families, hierarchical categorisation.
- Machine learning and neural networks applied to bioinformatics.

Learning activities and methodology

Title	Hours	ECTS	Learning outcomes
MOODLE activities	25	1	CM19, KM24, KM25, SM21, SM24
Study	10	0.4	CM19, KM24, KM25, SM21, SM24
Computer lab sessions	16	0.64	SM21, SM24
Tutorial sessions	6	0.24	CM19, KM24, KM25, SM21, SM24
Classroom sessions	10	0.4	CM19, KM25, SM24

Classroom sessions. These will cover the teoretical fundamentals of the course, and will be evaluated in the exam.

Autonomous learning- MOODLE activities. During the 8 weeks of the course, the instructor will propose several activities, to be performed autonomously. Students will deliver the outcome of these activities through the MOODLE platform. The activities proposed will range from visualisation and completion of tutorials, execution of procedures or questionnaires, depending on the subject matter. In general terms, activities will have a close relationship or will be complemetary to the problems and theoretical aspects of the computer lab and classroom sessions. It might be necessary that students perform a specific activity on MOODLE previously to a particular computer lab session, in order to fully benefit from it.

Autonomous learning: Study.

Computer lab sessions. These will be focused into the practical aspects of the course, and it is expected that students will become proficient in data search, procedural aspects and in the analysis of the information obtained by the predictors and databases covered throughout the lessons. The approach will be dynamic, and problems will be solved during the development of each session. Aspects covered in computer lab sessions will be evaluated in the exam.

Tutorial sessions. Individual or small group sessions, focused in doubts related to the course. Upon demand from students. Date/hour to be agreed with the instructor.

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

Continuous assessment activities

Title	Weight	Hours	ECTS	Learning outcomes
Exam, theoretical concepts	45%	2	0.08	CM19, KM24, KM25
MOODLE activities	10%	4	0.16	CM19, KM24, KM25, SM21, SM24
Exam, practical concepts	45%	2	0.08	KM24, SM21, SM24

There will be three different evaluation types:

1) Exams. There will be two exams. Each exam will evaluate theoretical and applied concepts respectively, covered during the sessions and can include: short questions, questionnaires or data analysis tasks or results proposed by the instructor. Each exam will contribute a 45% of the final mark, and will be solved individually by each student. In order to pass the exams, the mark must be equal or higher than 5/10 in each exam, and it will be possible to retake it at the programmed date at the end of the semester.

2) Delivery of tasks through MOODLE. All activities will weigh in total a 10% of the final mark. It will not be possible to retake any of them if they are delivered after the deadline or the student fails in any of them.

Each student must accomplish both the following criteria, in order to pass the course:

- a) Pass the exams with a mark that is equal or higher than 5/10 and,
- b) Obtain a mark that is equal to or higher than 5/10, after doing the weighted average of all four evaluation activities (exam, MOODLE, case study evaluated by instructor and by peers).

Retaking the exam and improving your mark

Those students who fail the exam can retake it on the planned date at the end of the semester. The text will have a similar format than the first exam. Those who wish to improve their marks can sit again for it, but specifically withdraw their former mark. In that case, the difficulty of the exam could be higher than for those students who failed. Students wishing to sit again for the exam must inform the instructor at least 48 h before the date, in order to plan the logistics (number of rooms needed, etc). Both exams will be revised on a date and place announced by the instructor, between 1 and 7 working days from the publication of the marks. Those students that are not able to attend the exam(s) due to a justified cause and provide the corresponding documentation to the Degree Coordinator, will have the right to sit for an exam on another date. The test might combine the resolution of problems with an oral exam. The Degree Coordinator will see for the practical implementation of that with the instructor. Any other aspect that is not specifically covered in this guide, will follow the general regulations for evaluation of the Bioscience Faculty. In order to retake the exam, students must have previously been evaluated in a set of activities that amount for two thirds of the total weight of the subject. Therefore, when evaluated activities are less than 67% of the total weight, the student will receive the "No Avaluable" mark.

This subject does not foresee the single evaluation or "avaluació única".

Any irregularity committed during an assessment activity (academic misconduct, plagiarism, or improper use of AI, unless such use is expressly authorized in the course syllabus) that may lead to a significant alteration of the grade will result in that activity being graded as 0. If the course syllabus stipulates that obtaining a

minimum mark in this assessment is an essential requirement to pass the course, or if multiple irregularities occur in the assessment activities of the same course, the final grade for the course will be 0. Furthermore, disciplinary proceedings may be initiated against any student who incurs any of these irregularities.

Bibliography

- Pevsner, Jonathan. 2015. Bioinformatics and functional genomics, 3rd edition. Wiley-Blackwel. ISBN: 978-1-118-58178-0.
- Lesk, Arthur. 2014. Introduction to Bioinformatics 4th edition. Oxford University Press. ISBN: 9780199651566.
- Pazos, Florencio; Chagoyen, Mónica. 2015. Practical protein bioinformatics. Springer international publishing. ISBN: 978-3-319-12726-2
- Web resources suggested by the instructor

Software

Programes:

Jalview: <https://www.jalview.org/>

MEGA X: <https://www.megasoftware.net/>

Notepad++: <https://notepad-plus-plus.org/downloads/c>

Icn3d: <https://www.ncbi.nlm.nih.gov/Structure/icn3d/icn3d-3.2.0.zip>

PyMol: <https://pymol.org/2/>

Pàgines web i Webservers:

<https://www.ncbi.nlm.nih.gov/>

<https://services.healthtech.dtu.dk/>

<https://www.expasy.org/>

<https://bio.tools/>

<https://www.ebi.ac.uk/services>

<https://alphafoldserver.com/>

<https://swissmodel.expasy.org/>

<https://search.foldseek.com/>

Course groups and languages

The information provided is provisional until November 30. After this date, you will be able to consult the language of each group through this [link](#). To access the information, you will need to enter the course CODE

Type of teaching	Group	Language	Semester	Shift
(TE) Theory	33	Catalan	second semester	morning-mixed
(PLAB) Practical	331	Catalan	second	morning-mixed

laboratories			semester	
(PLAB) Practical laboratories	332	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	333	Catalan	second semester	morning-mixed