Universidad Zaragoza

Academic Year/course: 2024/25

27123 - Bioinformatics

Syllabus Information

Academic year: 2024/25
Subject: 27123 - Bioinformatics
Faculty / School: 100 - Facultad de Ciencias
Degree: 446 - Degree in Biotechnology
ECTS: 6.0
Year: 3
Semester: Second semester
Subject type: Compulsory
Module:

1. General information

The objective of this subject is to introduce students to the use of basic bioinformatics tools and computational biology used in various fields of biotechnology. The course is taught in the second quarter of the third year , when students already have methodological and theoretical knowledge that makes them aware of the enormous amount of information to process when working with biological systems. The subject allows them to know and use the main databases of biomolecules and genomes, and to deepen in the search for information and its analysis. To take this subject, it is recommended to have taken Biochemistry, Molecular Biology and Structure of Macromolecules, as well as to have taken or to be taking Genetic Engineering at the same time.

These approaches are aligned with the following SDGs of the United Nations 2030 Agenda (https://www.un.org/sustainabledevelopment/es/), such that the acquisition of the subject's learning results provides training and competence to contribute to some extent to their achievement; Goal 3: Health and wellness; Goal 5: Gender equality; Goal 7: Affordable and non-polluting energy; Goal 9: Industry, Innovation and infrastructure; Goal 14: Underwater life; Goal 15: Life of terrestrial ecosystems.

2. Learning results

Upon completion of the subject, the student will be able to:

- Know, extract and use information from the main biomolecule and genome databases.
- Construct and interpret multiple sequence alignments.
- Construct and interpret phylogenetic trees.
- Perform basic analysis of protein and nucleic acid structures.
- Use computer tools to support diverse methodologies in Genetic Engineering and Structural Biology.
- Perform simple simulations of biomolecule interaction, quaternary organization prediction and homology modelling.
- Identify computational simulation methodologies in molecular dynamics analysis and in the study of enzymatic reactions involving biomolecules
- Use and read simple Python and networked collaborative notebook scripts.
- Tackle simple problems of molecular modelling, molecular dynamics, prediction of molecular interactions and prediction of catalysis using networked servers.
- Analyse and critically interpret the information obtained.
- Transmit in writing basic concepts of the methods studied and their application, as well as the results of a specific study
- Communicate conclusions.

3. Syllabus

MASTER CLASSES

1. Introduction.
2. Gene and protein sequence databases. Data entry and retrieval.
3. Sequence alignment.
4. Genome analysis and comparison. Metagenomes. Transcriptomics databases.
5. Metabolic pathway databases
6. Phylogenetic trees. Construction of distance matrices and cladograms.
7. Protein and nucleic acid structure databases. Data entry and applications of visualization.
8. Molecular simulation methods.
9. Molecular Dynamics and Monte Carlo.

10. Protein and nucleic acid structure prediction methods.

11. Molecular docking prediction methods (*docking*).

12. Simulation of biological reactions. Hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) methods.

13. Chemoinformatic: databases of organic molecules.

14. Tools for drug design. QSAR, ADMET.

15. Databases for proteomics and interactomics.

16. Databases and thematic servers (of diseases, etc.).

CASE STUDY CLASSES

Case 1: Sequence recovery, sequence alignment and construction of a phylogenetic tree.

Case 2: *In silico* gene amplification and cloning.

Case 3: Structural analysis: structure-function relationship of an enzyme.

Case 4: Molecular docking for drug design.

Case 5. Preparation of an analysis script. Analysis of a molecular dynamics trajectory.

PROJECT

Development of an individual tutored project on a real case and presentation of the results, discussion and conclusions in a report

4. Academic activities

MASTER CLASSES

Face-to-face. 2 ECTS. They present the basic theoretical knowledge of the subject. The basic material will be provided to students through UNIZAR's MOODLE blended learning platform.

CASE STUDIES

Face-to-face and mandatory. 2 ECTS. 5 sessions of 4 hours in a computer classroom. The student will be instructed on how to design their searches and simulations and interpret the results. The student will independently design searches, data analysis and simulations and critically evaluate the results obtained.

LEARNING THROUGH THE DEVELOPMENT OF AN INDIVIDUAL PROJECT

Face-to-face and mandatory. 2 ECTS. 5 sessions of 4 hours in a computer classroom for the preparation of a supervised project . Students will develop a specific tutored project and then generate a structured report including Results, Discussion, Conclusions, and Bibliography.

5. Assessment system

The general system will evaluate all the activities carried out by the student:

- **Theory exam.** Examination at the end of the term. It will include a multiple-choice test and another test to solve short theoretical questions and/or exercises. Usually: 50 multiple choice questions and 10 short questions (contribution to the grade 50/50% respectively). A grade of 5 out of 10 in each test is required for averaging. Exceptionally, students with a 4.5 grade in either of the two parts of the Theory exam and at least a 5.5 in the other may average both grades.
- **Practical Cases.** Continuous assessment **Attendance and completion are mandatory**. The student will write a report of each session that will be submitted through Moodle within one week from the end of the last face-to-face session. Only reports delivered in Moodle will be accepted. Those that are not delivered on time will not be eligible for a grade higher than 5 (out of 10) in the Practical Case.

6. Sustainable Development Goals

3 - Good Health & Well-Being
5 - Gender Equality
7 - Affordable and Clean Energy