Universidad Zaragoza

Academic Year/course: 2022/23

27123 - Bioinformatics

Syllabus Information

Academic Year: 2022/23
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

1.1. Aims of the course

The aim of this course is to introduce students to the use of basic bioinformatics and computational biology tools, familiarising them with their use in various fields of Biotechnology.

These approaches and objectives are aligned with the following Sustainable Development Goals (SDGs) of the United Nations Agenda 2030 (https://www.un.org/sustainabledevelopment/es/), so that the acquisition of the learning outcomes of the subject provides training and competence to contribute to some extent to their achievement.

- Goal 3: Health and well-being.

- Goal 7: Affordable and clean energy.

- Goal 9: Industry, innovation and infrastructure.

- Goal 14: Underwater life.

- Goal 15: Terrestrial ecosystem life.

1.2. Context and importance of this course in the degree

This subject is taught in the second semester of the third year of the Degree in Biotechnology and belongs to the Compulsory Training Module. At this point, students already have a large amount of methodological and theoretical knowledge, and are aware of the enormous amount of information that needs to be processed when working with biological systems.

This subject allows them to learn about the main databases of biomolecules, network servers for storage, information search or analysis. In the lectures and practical classes in the computer classroom, students will acquire basic knowledge and skills in this subject. With the elaboration of an individual personal project in the computer classroom, students will put into practice the knowledge acquired in a real case. This will allow them to work on transversal competences related to the search for information and its critical analysis, as well as in the writing and communication of scientific-technological contents.

1.3. Recommendations to take this course

In order to take this subject successfully, it is recommended to

* To have previously coursed Biochemistry, Molecular Biology and Structure of Macromolecules, as well as to have taken or to be taking Genetic Engineering at the same time.

* To carry out regular and continuous work throughout the course, actively participating in the theoretical and practical classes and tutorials, and carrying out the cases proposed in the computer room.

* To consult specific books related to the subject, in addition to the material provided by the lecturer.

2. Learning goals

2.1. Competences

On passing the course with flying colours, the student will be able to:

Identify the main databases of biological molecules available online. Obtain information from these databases (genomics,

transcriptomics, proteomics, metabolomics and other databases derived from massive analyses) and interpret it in biochemical and biotechnological terms.

Use basic bioinformatics tools for the analysis of macromolecule sequences and for phylogenetic studies.

Choose and use the appropriate tools to obtain structure-function data of a biological molecule from its sequence.

Use basic software to analyse macromolecule structures deposited in databases.

Tackle simple problems of molecular modelling, molecular dynamics, prediction of molecular interactions and prediction of catalysis mechanisms, using network servers.

Critically analyse and interpret the information obtained.

Transmit in writing basic concepts about the methods studied and their application, as well as the results of a specific study.

Communicate conclusions to specialised and non-specialised audiences in a clear and unambiguous way.

Have computer skills to obtain, analyse and interpret data, and to understand simple models of biological systems and processes at the molecular level.

To pose and solve questions and problems in the field of Biochemistry, Molecular Biology and Biotechnology through scientific hypotheses that can be empirically examined.

2.2. Learning goals

Know, use and extract information from the main biomolecule databases. Construction and interpretation of multiple sequence alignments.

Construction and interpretation of phylogenetic trees.

Carrying out basic analyses of protein and nucleic acid structures.

Use of computer tools in support of different methodologies of Genetic Engineering and Structural Biology.

Carrying out simple simulations of interaction between biomolecules, prediction of quaternary organisations and homology modelling.

Identification of computational simulation methodologies in the analysis of molecular dynamics and in the study of enzymatic reactions involving biomolecules.

Introduction to the use of simple Python scripts and collaborative network notebooks.

2.3. Importance of learning goals

The information derived from the use of different bioinformatics methods is essential for the management and analysis of data in areas involving living organisms, such as Biotechnology, Biochemistry, and Structural, Molecular and Cellular Biology. The competences that the student acquires in this subject will provide him/her with tools that will be of interest in the prediction and improvement of biological systems for their use in the different branches of Biotechnology**.**

3. Assessment (1st and 2nd call)

3.1. Assessment tasks (description of tasks, marking system and assessment criteria)

The student must demonstrate that he/she has achieved the expected learning outcomes by means of the following assessment activities

Theory exam at the end of the term. The specific competences will be assessed by means of written tests that will include a multiple-choice test and another one that will correspond to the resolution of short theoretical questions and/or exercises. Usually: 50 multiple-choice questions and 10 short questions (contribution to the mark 50/50% respectively). It will be essential to score 5 out of 10 in each of these tests in order for them to be averaged. This test will take place on the dates determined by the Faculty for this purpose during the official examination periods**.**

Practical Cases. Continuous assessment during the practical cases. Attendance and completion are compulsory. The student will prepare a short report of each practical session which will be submitted through the Moodle platform within one week of the end of the last classroom session. The deadline for submission of all reports will be 23:45 hours on the day set for each group. Only reports submitted through the Moodle platform will be accepted. Those that are not handed in on time via Moodle will not be eligible for a mark higher than 5 (out of 10) in the Practical Cases grade.

Preparation of an individual project. The rigour in obtaining results will be assessed, as well as the clarity and coherence in its presentation and discussion in the report to be submitted to the lecturer. The student will have one week after the end of the face-to-face sessions to submit the project through the Moodle platform. The deadline for submission of all reports will be 23:45 hours on the day set for each group. Only reports submitted through the Moodle platform will be accepted. Those that are not delivered on time through Moodle will not be eligible for a mark higher than 5 (out of 10) in the Practical Cases grade. Attendance and completion are compulsory.

General. Theory and Practicum (case studies + individual project) must be passed independently.

The following will contribute to the final grade of the course: Theory exam=50%, Practical Cases=20% and Individual Project=30%.

In order to pass this subject, it will be essential to have a 5 out of 10 in each of the computable sections, and 5 out of 10 in the overall grade.

Exceptionally, those students who obtain a 4.5 in one of the two parts of the Theory exam and at least a 5.5 in the other may average both marks. This average mark of the exam will be taken as the final mark of the course (independently of the mark

obtained in the Practical Cases and Individual Project, which must be passed in order to pass the course).

The Practical Cases and Individual Project grade only applies to the academic year in which they were taken, being the same for the June and September exams. If there is a new enrolment in the subject in a different academic year, they will have to be retaken.

Fraud or total or partial plagiarism in any of the assessment tests (including practical session reports) will result in failure of the subject with the minimum mark, in addition to the disciplinary sanctions that the guarantee committee adopts for these cases.

In addition to the aforementioned assessment method, those students who do NOT attend the compulsory practical sessions or do NOT submit the corresponding reports will have to take a **global test**, which will judge the achievement of the learning outcomes mentioned above. This test will consist of taking the Theory Exam on the same date and time as the rest of their classmates plus an additional test in the computer room on the dates determined by the Faculty for this purpose. These two evaluation tasks will contribute to the final mark 50%/50% respectively.

The syllabus that students must use to prepare for the different tests can be found in the "Programme" section of this teaching guide.

4. Methodology, learning tasks, syllabus and resources

4.1. Methodological overview

The methodology followed in this course is oriented towards the achievement of the learning objectives. A wide range of teaching and learning tasks are implemented, such as theory sessions, informatic lab sessions and assignments.The learning process is designed so that on the basis of an intensification of the theoretical knowledge the students will be able to acquire an orientation in the management of bioinformatic tools that is eminently practical and applied in the computing room.

Students are expected to participate actively in the class throughout the semester, particularly in the computer lab. As far as possible students will be able to choose the bioinformatic tools to apply for particular needs on the basis of theoretical and practical knowledge. In this strategy the realization of general practical cases allows the student to become familiar with diverse on-line bioinformatics tools, to subsequently move to the resolution of a real biochemical problem that, ultimately, is the applied section and a way to approach the students to day-to-day work situations.

Thus, the subject has an applied orientation, the proposed activities are focused in the application of a series of principles first to concrete cases, through the analysis and results interpretation of cases provided by Professor, and them by the individual preparation of a supervised but real case requiring the application of one or more of the methodologies treated in the course.

Classroom materials will be available via Moodle. These include a repository of the lecture notes used in class, the course syllabus, as well as other course-specific learning materials. Further information regarding the course will be provided on the first day of class.

4.2. Learning tasks

The course includes the following learning tasks:

- LECTURES (2 ECTS). Face-to-face. 20 hr. Basic theoretical knowledge of the subject is presented. Computer screen projections, including animations, videos and navigations online will be used. The basic material will be provided by the professors to the students through the MOODLE UNIZAR learning platform.
- PRACTICE CASE STUDIES (2 ECTS). Face-to-face and mandatory. 20 hours. Computer room. The professor will distribute practical cases through the online learning platform, and he will instruct the students in how to design their searches, simulations and interpret the results. These activities will help the student to acquire the capacity and skills to later analyze and solve particular problems by hisowm/herowm. The student will be able to independently design searches, data analysis and simulations and to critically evaluate the results obtained.
- ASSESSMENT TASK. Face-to-face and mandatory. 20 h. 5 sessions of 4 hours in the computer classroom were the professor will assist the students to prepare an individual project. The students will develop a concrete case on an individual basis and then generate a report, for evaluation, according to the extension and regulations indicated in the directions provided by the professor. The analysis of the information should lead to the preparation of a structured presentation that must contain results, discussion, conclusions, and bibliography sections. This activity will encourage students to use various software applications and servers, which have been explained in the theoretical classes and used in the sessions of practical cases, to resolve a particular problem. This activity stimulates the use by students of online scientific material as well as its interpretation, communication and discussion.

"Teaching and evaluation activities will be carried out in face-to-face mode, unless the rules issued by the competent authorities and the University of Zaragoza have them carried out on-line."

4.3. Syllabus

The course will address the following topics:

1. Introduction.

2. Sequence Databases: genes and proteins. Data introduction and recovery.
3. Sequence alignment.
4. Analysis and comparison of genomes. Metagenomes. Transcriptomics data bases.
5. Metabolic pathways databases.
6. Phylogenetics.
7. Proteomics and interactomics databases.
8. Protein and nucleic acid structure databases. Introduction of data, and applications for visualization.
9. Cheminformatics: small molecule databases.
10. Tools for drug design. QSAR, ADMET.
11. Thematic databases and servers.
12. Methods for Molecular Simulation.
13. Molecular Dynamics and Monte Carlo.
14. Protein and nucleic acid structure prediction methods.
15. Molecular docking.
16. Hybrid Quantum Mechanics/Molecular mechanics (QM/MM) Methods. Simulation of enzyme reactions.

PRACTICE CASE STUDIES will address the following topics:

Case of study (20 hours), Computer room.

- Case 1: Recovery of sequences, sequence alignment and phylogenetic tree construction.
- Case 2: In silico gene amplification and cloning.
- Case 3: Structural analysis: enzyme structure-function relationships.
- Case 4: Protein-ligand docking.
- Case 5. Preparation of an analysis script. Analysis of a molecular dynamics trajectory.

ASSESSMENT TASK

Project (20 hours), Computer room.

Individual project applying learned methods. Each student will present a report of his/her project following the guidelines given in the corresponding protocol.

4.4. Course planning and calendar

Schedules of lectures and problems will coincide with the officially established and will be available at: https://ciencias.unizar.es/grado-en-biotecnologia.

The places, calendar and groups for training and practical sessions will be established in coordination with the rest of subjects at the beginning of course. The Coordinator will produce the groups of students for these activities at beginning of course to avoid overlaps with other subjects.

The course will begin with the 20 hours of lectures session (February-March). Then there will be a week of practical cases with 5 cases in the computer room in 5 sessions of 4 hours each (February-April).

Finally students will benefit from another week of 5 sessions of 4 hours in the computer room for the preparation of the individual project assisted by the teacher, and then of an additional week for completion by their owns (April-May).

For students enrolled in the subject, places, times and dates of lectures and practical sessions will be public via Bulletin Board advertisements of the grade on the platform Moodle at the University of Zaragoza, https://moodle2.unizar.es/add/, and in the moodle page for the course. These routes will be also used to communicate enrolled students their distribution by groups of practical sessions, which will be organized by the coordination of degree. Provisional dates will be available on the website of the Faculty of Sciences in the corresponding section of the Degree in Biotechnology: https://ciencias.unizar.es/grado-en-biotecnologia.

In this web there will be also available the dates of exams.

4.5. Bibliography and recommended resources

Recomended Text Books can be found at

http://psfunizar10.unizar.es/br13/egAsignaturas.php?codigo=27123