



UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Strutture e Interazioni Molecolari

2627-2-F5402Q031

Aims

The course is aimed at providing the theoretical and practical basis of bioinformatics and computational methods to study structure-function relationships in biological macromolecules and metabolic networks.

At the end of the course students have acquired the theoretical bases of the main computational and bioinformatics methods suited to study structure-activity relationships and will be able to use software to study structure-activity relationships in biomolecules and metabolic networks, as well as discuss critically results.

Knowledge and understanding

The student will gain knowledge about theory and computational methods to study structure-function relationships in biomolecules.

Applying knowledge and understanding

The student will be able to apply the knowledge acquired under 1. to the subsequent subjects.

Making judgements

The student will be able to process the acquired knowledge towards its application in topics related to structure-function relationships in biomolecules.

Communication skills

Use of an appropriate scientific/chemical vocabulary and ability in oral reports

Critical and judgment skills

Case studies related to computational applications in industrial biotechnology will be examined together with the students.

Learning skills

Skills in reading and understanding the subsequent studies requiring knowledge of structure-function relationships theory and methods.

Contents

Computational methods to query biological databases. Analysis and comparison of protein sequences. Homology modelling, fold recognition and ab initio methods to predict protein structures. AI-based computational methods for predicting the structural and functional properties of biomolecules.

Molecular mechanics and molecular dynamics.

Molecular recognition: protein-ligand and protein-protein interactions.

Biotechnological application of metalloenzymes in energy and bioremediation fields.

Computational methods for the analysis, modelling and reconstruction of metabolic networks.

Detailed program

Query of databases containing protein sequences and structures.

Basic notions about protein sequence alignments. Score matrices.

Homology, similarity and identity.

BLAST and FASTA. Clustal.

Introduction to the experimental methods to derive the three-dimensional structure of proteins.

Theoretical bases of computational methods used to predict protein structures. Homology modelling. Fold recognition.

Ab initio methods to study structural and functional properties of proteins.

AI-based computational methods for predicting the structural and functional properties of biomolecules.

Methods to validate protein structures.

Molecular mechanics and dynamics.

Ligand-based and receptor-based methods in virtual high throughput screening.

QSAR and machine learning.

Docking methods.

Biotechnological applications of enzymes in energy and bioremediation fields.

Computational methods to study metabolic networks. Metabolic Control Analysis and Flux Balance Analysis.

Laboratory sessions where computational and bioinformatics tools are used to:

- Design enzyme variants
- Predict protein structure
- Study structure-function relationships in metabolic networks.

Prerequisites

Background. Basic knowledge of biology, chemistry and physics.

Prerequisites. None

Teaching form

24 2 hours-lectures in person delivered didactically (Didattica erogativa, DE) focused on the presentation-illustration of contents by the lecturer.

20 hours of in person Tutorial computational activities aimed at guiding and assisting students throughout their studies in view of the exam preparation delivered by interactive teaching (Didattica Interattiva, DI) through in-person tutorials.

All lessons are recorded and made available on the corresponding e-learning web page.
Lessons are in Italian.

Textbook and teaching resource

Slides. Available at the e-learning platform of the course.

Bibliography. Selected scientific papers and reviews available at the e-learning platform of the course.

Semester

First semester

Assessment method

The student obtains the course credits (CFU) by passing an oral examination. No in-course assessments are planned.

The oral examination, graded on a scale of 30, consists of an interview in which the student must respond clearly and using appropriate language to open questions relating to the topics and issues covered during the lectures. The final grade will be determined according to the following scale:

18–21: preparation covering a limited portion of the course syllabus, with weak ability to independently discuss and analyse topics, which in the oral exam emerges only following the instructor's guidance and prompting; sometimes uncertain presentation skills, with language that is not always clear or precise and occasionally incorrect, and very limited critical thinking ability.

22–24: preparation covering a good number of the topics included in the course syllabus, although not in a fully balanced way, with sufficient ability to independently discuss and analyse topics, sometimes supported by the instructor's questions; reasonably clear presentation skills, generally correct vocabulary, although at times not precise or clear, and limited critical thinking ability.

25–27: preparation covering a wide range of topics included in the course syllabus, with good autonomy in argumentation and critical analysis, and the ability to apply knowledge to concrete cases; correct use of vocabulary and good command of disciplinary language.

28–30/30 with distinction (30L): comprehensive and exhaustive preparation on the course syllabus topics, strong autonomous ability in discussion and critical analysis of the topics, ability to connect themes to concrete cases and to different contexts and disciplines, excellent critical and independent thinking skills, full command of disciplinary terminology, rigorous and well-structured presentation skills, and strong argumentative ability.

Office hours

Contact Monday 15.30-17.30

Sustainable Development Goals

RESPONSIBLE CONSUMPTION AND PRODUCTION
