UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

# SYLLABUS DEL CORSO

## Strutture e Interazioni Molecolari

**2425-1-F0802Q040**

### Aims

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

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.
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.
Metods 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 didactics (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.

## 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.

Textbooks
Stefano Pascarella, Alessandro Paiardini, Bioinformatica -Dalla sequenza alla struttura delle proteine, 2010, Zanichelli

## Semester

First semester

## Assessment method

Oral examination where the topics of the course are discussed from both a theoretical and practical standpoint, with a specif focus on biotechnological applications.

## Office hours

Contact Monday 15.30-17.30

## Sustainable Development Goals

RESPONSIBLE CONSUMPTION AND PRODUCTION