BIO-315 **Structural biology**

Dal Peraro Matteo

Cursus	Sem.	Type
Computational science and Engineering	MA2, MA4	Opt.
Computational science and engineering minor	E	Opt.
Life Sciences Engineering	MA2, MA4	Opt.
Minor in life sciences engineering	E	Opt.
Physics of living systems minor	E	Opt.

Language of teaching	English
Credits	4
Session	Summer
Semester	Spring
Exam	During the semester
Workload	120h
Weeks	14
Hours	**4 weekly**
Lecture	2 weekly
Exercises	2 weekly
Number of positions	

Summary

The main focus of this course is on the molecular interactions defining the structure, dynamics and function of biological systems. The principal experimental and computational techniques used in structural biology, as well as molecular modeling and design will be introduced and practiced.

Content

The course will focus on the following topics:
1. Structure: intermolecular interactions, structure of biomolecules, experimental methods in structural biology (i.e., X-ray crystallography, NMR, cryo-electron microscopy), structural classification, protein structure prediction using genomic data and machine learning.
2. Dynamics: elements of statistical mechanics, molecular mechanics of biomolecules, molecular simulations, molecular binding and free energy calculations.
3. Selected topics: protein design and engineering; protein folding, molecular docking, integrative modeling; structure-based drug discovery, machine learning for structural biology.
Practicals and projects will run in parallel to lectures to have a first-hand experience on molecular visualization, major structural biology techniques, molecular modeling, protein design, biomolecular mechanics and dynamics, structure-based drug design, protein interaction networks, macromolecular assemblies, protein structure predictions using AlphaFold.

Keywords

Structural biology, X-ray crystallography, cryo-EM, NMR, AlphaFold, SAXS, integrative modeling, molecular modeling, molecular mechanics, molecular simulation, protein structure prediction, protein folding, protein design, drug discovery, machine learning.

Learning Prerequisites

Required courses

None in particular, but some are recommneded (see below)

Recommended courses

Basic bachelor courses on Maths, Physics, Molecular Biology and Biochemistry

Important concepts to start the course

Structural biology and biochemistry of biomoleculaes. Classical mechanics, themodynamics, and

electrostatics (Physics I, II, III), Organic Chemistry.

Learning Outcomes

By the end of the course, the student must be able to:

- Explore the structure of biomolecules (and their interactions)
- Predict the structure and dynamics of proteins
- Design the structure of proteins
- Visualize biomolecules
- Interpret structural data
- Choose the appropriate method to tackle a problem
- Design a project in structural biology
- Make a scientific report and presentation

Transversal skills

- Make an oral presentation.
- Write a scientific or technical report.
- Use a work methodology appropriate to the task.
- Demonstrate the capacity for critical thinking
- Use both general and domain specific IT resources and tools

Teaching methods

Half of the course is based on lectures, while in the other half practical experiences and projects (computational and experimental) are provided to the students.

Expected student activities

Attending lectures, completing practical experiences, reading assignments, presenting a scientific paper, developing a project, writing a report, presenting the results of a project

Assessment methods

Assignments and projects assessment during the semester

Supervision

Office hours	Yes
Assistants	Yes
Forum	Yes

Resources

Moodle Link

- https://go.epfl.ch/BIO-315