

BIO-315

**Structural biology**

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<b>Cursus</b>	<b>Sem.</b>	<b>Type</b>
Biocomputing minor	E	Opt.
Computational science and Engineering	MA2, MA4	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
<b>Hours</b>	<b>4 weekly</b>
Lecture	2 weekly
Exercises	2 weekly
<b>Number of positions</b>	

**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 recommended (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 biomolecules. Classical mechanics, thermodynamics, 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>