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

Content
2. Dynamics: elements of statistical mechanics, molecular mechanics of biomolecules, molecular dynamics simulations, binding and free energy calculations.
3. Selected topics: de novo protein structure prediction and design; protein folding, molecular assembly and misfolding; structure-based drug discovery, multiscale molecular simulation techniques.

Practicals and projects will run in parallel to lectures to have a first hand experience on molecular visualization, X-ray crystallography, molecular modeling tools applied to protein structure prediction, biomolecular mechanics and dynamics, structure-based drug design.

Keywords
Structural biology, X-ray crystallography, integrative modeling, molecular modeling, molecular mechanics, molecular simulation, protein structure prediction, protein folding and design, drug discovery.

Learning Prerequisites
Recommended courses
Basic bachelor courses of Mathematics, Physics, Molecular Biology and Biochemistry

Important concepts to start the course

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 of proteins
• Work out / Determine the structure of biomolecules
• Perform X-ray crystallography experiments
• Perform molecular modeling and simulation
• Choose the appropriate method to tackle a problem
• Design a project in structural biology
• Make a scientific report and presentation
• Assess / Evaluate the role of intermolecular interactions in biology

Transversal skills
• Set objectives and design an action plan to reach those objectives.
• Assess one’s own level of skill acquisition, and plan their on-going learning goals.
• Assess progress against the plan, and adapt the plan as appropriate.
• Continue to work through difficulties or initial failure to find optimal solutions.
• Use both general and domain specific IT resources and tools
• Make an oral presentation.
• Write a scientific or technical report.

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, doing a project, writing a report, presenting the results of a project

Assessment methods
Projects assessment during the semester

Supervision
Office hours     Yes
Assistants      Yes
Forum           Yes

Resources
Bibliography
Molecular modelling: principles and applications, A.R. Leach, Pearson
Molecular modeling and simulations, T. Schlick, Springer

Ressources en bibliothèque
• Molecular modeling and simulations / Schlick
• Molecular modelling / Leach

Notes/Handbook
Lecture slides and exercises are provide via moodle.

Moodle Link
• http://moodle.epfl.ch/enrol/index.php?id=6741