



# Full Syllabus



<b>Course Title</b>	
Computational Structural Biology	
<b>Lecturer</b>	
Pr. Nir Ben Tal, Dr. Jérôme Tubiana	
<b>Semester</b>	
ב	
<b>Course requirements</b>	
<ul style="list-style-type: none"> <li>• <b>Prerequisites for CS/engineering students:</b> Prior biological background is valuable but not necessary, as the main biological concepts will be introduced in class.</li> <li>• <b>Prerequisites for Life Science / Med students:</b> Prior knowledge of Python (e.g. an introductory Coursera course or course 0455-1819) is valuable as we will study Python codes in class. However, <b>programming is not necessary to complete the assignments.</b></li> </ul>	
<b>Final grade components</b>	
Grade = 0.25 * home_exam_grade + 0.75 * project_grade + Mandatory home assignments.	
<b>Course schedule</b>	
<b>Class no.</b>	<b>Subject and Requirements (assignments, reading materials, tasks, etc.)</b>
Classes 1,3 17/03, 24/03	Introduction to Proteins and Structural Biology.
Class 2 20/03	Alignments of biological sequences: Pairwise & multiple alignments; Substitution Matrices; Dynamic Programming.
Class 4 27/03	Molecular visualization, Uniprot and PDB
Class 5 31/03	Homology Search: BLAST/MMSeqs; pHMMs; paired MSAs.
Class 6 03/04	Experimental Structure Determination Protein Sequence analysis with Python
Classes 7&8 07/04; 08/04	Alignments of Protein Structures: RMSD & Kabsch algorithm; TM-Score and TM-Align; Sequence order-independent Alignments; FoldSeek.
Classes 9 & 10 21/04; 24/04	Prediction of Protein Structures: Homology modelling; Coevolution; Contact map prediction with Direct Coupling Analysis and Convolutional Neural Networks (AlphaFold1).
Classes 11 & 12 28/04; 01/05	Molecular Energetics; Force Fields; Prediction of Protein Motion (Molecular Dynamics). Prediction of Protein-Ligand interactions (Small Molecule Docking).
Classes 13 & 14 05/05; 08/05	Prediction of Protein Structures and complexes: AlphaFold2 and 3. Protein Language Models.



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Class 15 & 16 12/05 & 15/05	Nucleic Acids structure theory and prediction.
Class 17 19/05	Protein Function Prediction (Gene Ontology terms / EC numbers).
Class 18 22/05	Computational Protein Design #1: Background; Fixed-backbone design with Rosetta; Inverse Folding Graph Neural Networks Generative Models (ProteinMPNN).
Class 19 29/05	Presentation of real-world use cases of the tools studied.
Class 20 05/06	Prediction of protein motion (Normal Mode Analysis)
Class 21 09/06	Computational Protein Design #2: Structure Generative Models (Diffusion Generative Models; Binder Design).
Classes 22 12/06	Tutorial on Computational Binder Design Guest lecture on real-world use cases of protein design.
Class 23 16/06	Missense Variant Effect Prediction (ClinVar, MSA-based, supervised, AlphaMissense)
Class 24 19/06	Tutorial on Protein Engineering; Selected Research Topics
Classes 25-26 23/06; 26/06	Selected Research Topics

## Required course reading

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## Optional course reading

- Introduction to Proteins: Structure, Function and Motion, Kessel and Ben Tal, 2018

## Comments

- The course is taught in English.
- The course is open to Life Science, Computer Science, Physics, Chemistry, Engineering (bioengineering) and Medicine students.