TEL AVIV UNIVERSITY
אוניברסיטת תל אביב

Full Syllabus

Course Title

Computational Structural Biology

Lecturer

Pr. Nir Ben Tal, Dr. Jérôme Tubiana

Semester

ב

Course requirements

- **Prerequisites for CS/engineering students**: Prior biological background is valuable but not necessary, as the main biological concepts will be introduced in class.
- **Prerequisites for Life Science / Med students:** 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, **programming is not necessary to complete the assignments.**

Final grade components

Grade = 0.25 * home_exam_grade + 0.15 * homeworks + 0.6 * project_grade

Course schedule

Class no.	Subject and Requirements (assignments, reading materials, tasks, etc.)
Classes 1-2	Introduction to Protein Structures; Forces and interactions.
Classes 3-4	Alignments of biological sequences (Pairwise & multiple alignments; Substitution Matrices; Dynamic Programming).
Classes 5-6	Homology Search (BLAST/MMSeqs; pHMMs; FoldSeek; paired MSAs).
Class 7	Prediction of Protein Structures #1: Homology modelling & Threading.
Classes 8-9	Alignments of Protein Structures (Kabsch algorithm; TM-Align; Sequence order-independent Alignments).
Class 10	Prediction of Protein Structures #2: Coevolution models (Direct Coupling Analysis)
Class 11	Prediction of Protein Functional Sites (ConSurf)
Class 12	Prediction of Protein-Ligand interactions (Small Molecule Docking).
Class 13	Prediction of Protein Motion (Normal Mode Analysis; Molecular Dynamics)
Class 14	RNA structure prediction and analysis.
Class 15	Prediction of Protein Structures #3: Deep Convolutional Neural Networks (AlphaFold1).
Classes 16-17	Computational Protein Design #1: Background; Fixed-backbone design with Rosetta; Inverse Folding Graph Neural Networks Generative Models (ProteinMPNN).
Classes 18-19	Protein embeddings (Protein language models) & Protein Function Prediction (Gene Ontology terms).
Classes 20-21	Prediction of Protein Structures #4: AlphaFold2-3.

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Class 22	Computational Protein Design #2: Structure Generative Models (Diffusion Generative Models; Binder Design).
Classes 23-24	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, Engineering (bioengineering) and Medicine students.