UNIVERSITÀ DEGLI STUDI DI MILANO

Structural Bioinformatics

Carlo Camilloni

Time table: please note the change of venue

ONLY Tuesday 8, October 14.30-17.30: room 305

ALL OTHER Tuesday 14.30-17.30: Computer room at the Department of Biosciences, if you have never been there, go before the next week to register an account (if you want to use the local machines).

Friday 13.30-15.30: room 402

Course Material

ARIEL is available for course communications

All teaching material is available from GitHub:

https://github.com/carlocamilloni/Structural-Bioinformatics

- **Slides**
- **Practicals**
- **Review papers**
- **Exam papers (to be updated)**

All this material is part of the EXAM

Exam: something new

Make a presentation (~10 min) to discuss a scientific paper from a list I will share at the end of the course.

Most questions will be on those techniques employed in the paper you chose and that have been presented in the lectures.

Half of your final grade:
Contribute to the presentation of 2 reports of practical activities (these will happen on Tuesday lectures)

Or

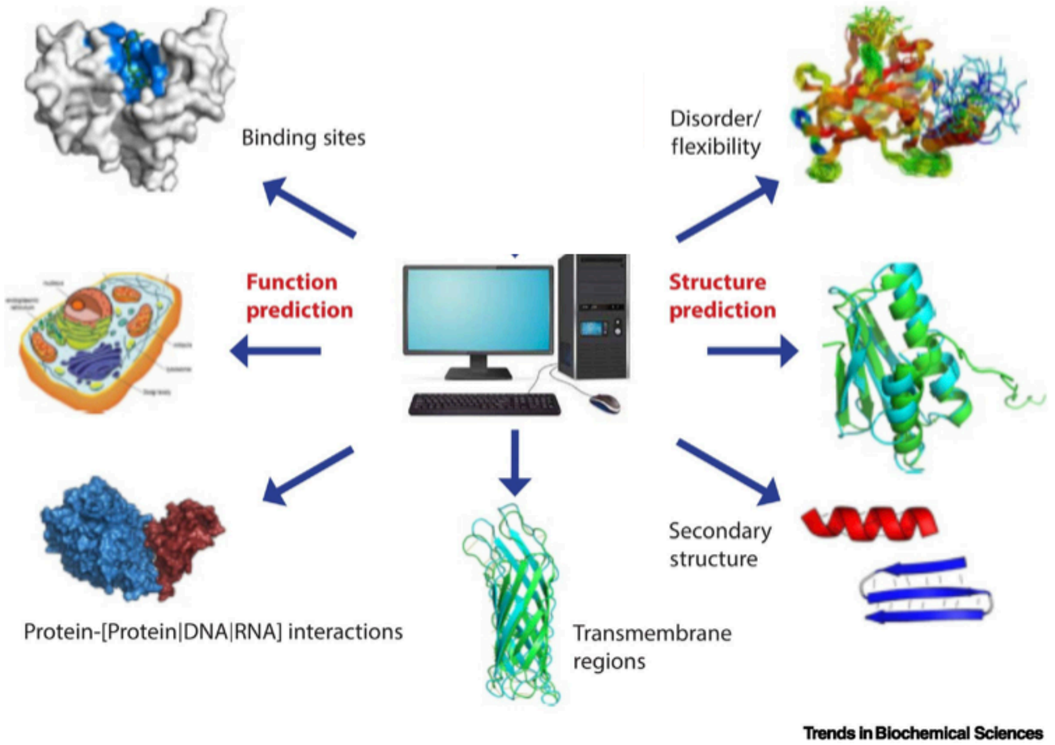
Have all the reports at the exam and discuss two of them.

Structural Bioinformatics

Nowadays SB covers a number of different topics that involve the structure of biomolecules and the use of computers to study them:

- How to predict the structure of biomolecules (proteins, but also nucleic acids, complexes, etc.)
- How to study their function and/or disfunction including the effect of mutations, partners, environment
- How to design new biomolecules

SB inherits from statistical methods, physics, chemistry, biochemistry and structural biology.



Bordin, N. *et al*. Novel machine learning approaches revolutionize protein knowledge. *Trends Biochem. Sci.* **48**, 345–359 (2023).

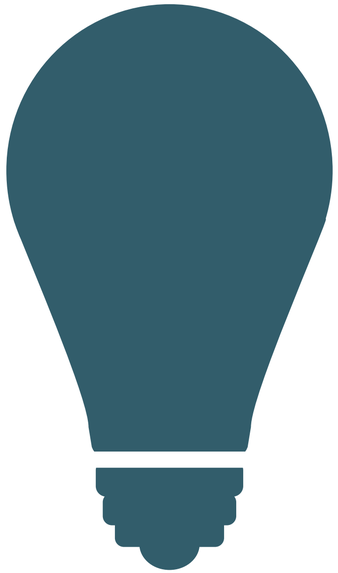
Aims and Background

- **Have a general understanding of what you can do with computer modelling (what kind of problems can be addressed and how?)**

- **Have a general understanding of the theoretical concepts that are the foundation of the field (why things work?)**

- **Know what are the strengths and weaknesses of different methodologies (What is the right method for a given problem and what are the limitations?)**

- **Have the tools to read and understand the scientific literature of the field**



Program

1. **Structural Biology and Visualisation**
2. **Statistical Picture of Biomolecules: theoretical framework**
3. **Classical Molecular Dynamics**
4. **Enhanced Sampling Techniques**
5. **Markov State Models**
6. **Quantum Chemistry and Simplified Models**
7. **Machine Learning**
8. **Structure Prediction and Molecular Docking**
9. **Integrative Modelling and Protein Design**

Topics will be both introduced theoretically
and practised hands-on

Practicals

Install VMD (version 1.9.4) if you will use your own laptop

https://www.ks.uiuc.edu/Research/vmd/

We are going to use COLAB: colab.research.google.com

To use them (essentially to save the results of your work)
You need a google Drive account, please activate one

You should work in small groups (two/three).

Reports should be produced summarising all activities