SAPIENZA
UNIVERSITÀ DI ROMA

Dottorato di Ricerca
in Biochimica

Dottorato di Ricerca in Biochimica
Scuola di Dottorato in Biologia e Medicina Molecolare
Corso di Bioinformatica Teorico-Pratico 6° Edizione

" BIOINFORMATICS: THEORY AND APPLICATIONS FROM GENOMES TO DRUGS"
6° Edition

- **CFU: 3 (20 hours of theoretical-practical lectures, plus one specialized seminar)**

Teachers

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Location

Computer Room C1 of the Department of Biochemical Sciences "A. Rossi Fanelli", Sapienza University of Rome (see map, building n. CU010, 2nd floor)

Calendar

From June 4th to July 4th: every Monday and Wednesday, from 2:30 to 4:30 pm
Starting lecture: June 4th 2018 at 2:30 p.m.

Application Guidelines

The course is addressed to 2nd year students of the BeMM Ph.D. School and can host a maximum of **30** students. Applications should be sent by e-mail to francesco.malatesta@uniroma1.it, not later than **May 31st 2018**. Please, indicate "Bioinformatics Course" as the e-mail object, and your Surname and Name, as well as the title of your Ph.D. course, in the text body. ***Student selection will be based on time of arrival of the application***. Selected students will be notified by e-mail, and should guarantee their attendence. Certificates of participation will be issued to students who have acquired at least 2/3 of the total lectures.

Aim of the Course

- Participants will learn the principles of gene/protein evolution, which constitute the theoretical basis of fundamental approaches to the study of proteins and nucleic acids.
- Participants will be presented with a range of Bioinformatics techniques most commonly employed in the computational study of proteins and nucleic acids; about half of the course is dedicated to the practical use of these techniques.
- In particular participants will acquire basic knowledge on how to analyse protein and nucleic acid sequences and protein structures, predict three-dimensional protein structures, and rationally design small molecule drugs
- By the end of the course, participants will be able to rationally use, and interpret results of, standard methods presented in the course; importantly, they will gain a deeper understanding of what biological problems can be best tackled by computational methods.
- Finally, participants will be provided with fundamental knowledge and material for further personal studies.

Detailed program

1. Molecular Evolution: Why is it Important?

- Homology vs. sequence, structure and function similarity
- Relationship between protein sequence identity and similarity in structure and/or function

2. The World Wide Web: An infinite Source of Precious (and Rubbish) Information

- Separate the wheat from the chaff: reliable resources (Nucleic Acids Research; NCBI; EBI; UniProt; ExPASy; PDB; GO)

3. Protein Sequence Analysis: What can it tell us?

- Knowledgebases (UniProt, NCBI Gene): function, interactions, intracellular compartment
- Sequence comparison and database search: pairwise vs. profile-based methods (Blast; Psi-Blast); % sequence identity and E-value; sequence similarity; insertions and deletions
- Multiple sequence alignments and phylogenetic trees

4. Sequence-based Predictions

- domains: building blocks of large proteins
- globular vs. disordered proteins (domains); membrane or not membrane; signal peptides; secondary structures
- modifications post-translation: phosphorylation, glycosylation, ubiquitination;
- handy tools from ExPasy: amino acid composition; isoelectric point; molecular weight; hydrophobicity; cleavage sites; one-letter to three-letters and back; motif identification

5. Protein Structure Prediction: Are We Solving the Folding Problem?

- protein 3D structures can be visualized in a variety of ways (PyMol)
- protein structures can be compared (CE)
- protein structures can (often) be predicted:
    - Homology Modelling (Modeller, PyMod)
    - Fold Recognition (Phyre; PsiPred)
    - "De novo" predictions (Rosetta/Robetta)

6. Interacting with Protein Structures

- Docking small molecules to protein functional sites
- Pharmacophore screening and rational drug design

7. A big, big world: an overview of "Omic" disciplines and "high-throughput" data

- Genomics and transcriptomics
- Epigenomics

8. NGS and Exome Sequencing

- Advanced approaches to study the molecular basis of mendelian disease

Specialized Seminar

Friday, May 25th 2018 at 12:00 in Room B of the Department of Biochemical Sciences "A. Rossi Fanelli", Sapienza University of Rome (building CU010, first floor, see map)

Prof. Leonardo Guidoni (University of L'Aquila): "Atomistic Simulations In Biochemistry: Molecular Details Of The First Steps In Photosynthesis"