Summer Seminars on Computational Biochemical Tools and Methods

The Institute of Biosciences – University Research Center of Ioannina (I.B.S.-URC-Ioannina) organizes a seminars cycle on Molecular Docking, Protein Structure Prediction, and Computational Toxicology.

The Director of the I.BS.-URC-Ioannina announces the conduct of an educational seminar series for undergraduate and postgraduate students at the University of Ioannina on Computational Biochemistry with emphasis on **molecular docking** the **prediction of protein structure based on artificial intelligence,** and **computational toxicology**. In these seminars, students will be trained in basic knowledge of molecular docking, use of alpha fold, and toxic risk assessment, and learn to use state-of-the-art software based on open-source code that will be used for all three subject areas. A prerequisite for participation in the seminar series is the knowledge of basic concepts of biochemistry and the comfortable use of a computer.

The seminars will consist of:

- Molecular docking (Introduction, molecular docking methods, comparison of the methods, use of visualization tools and docking software: autodock vina, autodock tools, pymol. Various other software tools will be presented.
- Analysis and use of the "Alphafold" artificial intelligence system.
- Introduction to computational toxicology and vega software.

Program

	29/08/2022	30/08/2022	31/08/2022	01/09/2022	02/09/2002
9:00-11:00	Introduction to molecular docking	hands-on training	Protein folding and artificial intelligence	hands-on training	Introduction to Computational toxicology, Smiles representation of molecules Vega software
11:30-13:00	autodock tools -autodock vina - pymol	hands-on training	Alphafold	hands-on training	hands-on training

Instructor

Dr. George Papamokos University of Ioannina

Dr. George Papamokos is a research associate at the University of Ioannina - Department of Physics and Medicine, also affiliated with the Physics Department of Harvard. His expertise lies in Computational Biochemistry and Soft matter, particularly in Epigenetics, Computational Toxicology, and modeling-characterization of new materials.

Registration

To register, please send an email to the following email address:

gpapamokos@uoi.gr

The registration deadline is July 26th 2022.

The email will include your name, student registration number, and the Department to which you belong.

The seminars are free of charge. There are **12 seats** available.
As far as **undergraduates** are concerned, priority will be given to students who already have work related to the seminar subjects.
Regarding **postgraduate students**, priority is given to students working in biochemistry and molecular biology laboratories, and their supervisors are interested in introducing computational tools to their research.
The committee for the selection of applicants consists of the following members:

Prof. Stathis Frillingos, Biol. Chem. Lab, Dept. of Medicine, UoI; Director of I.BS.-URC-Ioannina;
https://urci.unit.uoi.gr/ibs/en/contact.html
http://www.frillingoslab.gr/

Assoc. Prof. Anastasia Politou, Biol. Chem. Lab, Dept. Medicine, UoI; Inst. Biomed. Res.-FORTH
https://www.bri.forth.gr/bri-people/en/politou-laboratory

Dr. George Papamokos, Research Associate, Dept. Physics and Medicine, UoI
http://softmatter.physics.uoi.gr/node/9
https://www.bri.forth.gr/bri-people/en/politou-laboratory

The seminars will be implemented in the University of Ioannina Computer Room in the "Metavatiko" building.

Seminars

Molecular Docking

Molecular docking is a prerequisite for drug design to identify fundamental interactions between two molecules, usually between the protein molecule and the drug. Yet, this method is attributed to many irreproducibility problems in medicinal chemistry and pharma. In this seminar, we will explore the different approaches to molecular docking and recent strategies that make molecular docking more reliable.

Alphafold

Protein folding was an unsolved problem for more than 50 years until recently. An AI system solved it based on machine learning techniques and the available protein structures in the PDB database. In this seminar, I will present the alphafold architecture, and we will learn to use it in various case studies. Finally, we will assess its usage and test its limits of accuracy.

Computational Toxicology

Computational toxicology provides predictive tools for the properties of chemical compounds: carcinogenicity, hepatotoxicity, cardiotoxicity, renal toxicity, genotoxicity, phototoxicity, metabolites, idiosyncratic toxicity models, and software tools, to name a few of them, are currently available to assist the toxicological assessment of chemicals. In this seminar, you will be introduced to toxicology and its computational tools and learn to use the vega software and the smiles language.

Envoy

"Today, the computer is just as important a tool for chemists as the test tube. Simulations are so realistic that they predict the outcome of traditional experiments."[1]

[1] Nobel Prize in Chemistry announcement 2013