Postgraduate student: **Manoussidou Theodora**

Thesis Title:

Evaluation and comparison of bioinformatics tools for studying 3d protein structure

Abstract:

The subject of this thesis project is related to the geometrical representation of molecular structures in the three-dimensional space, as it is being carried out by different Bioinformatic tools. The main addressed goal is the comparative study of these tools, regarding the accuracy of their predictions and their ability to map the various binding sites that can be found on the targeted molecules.
The structure of Glycogen Phoshorylase, that has been extensively used as a molecular target in the process of drug design, for the study against the disease of Diabetes 2, was used as a control.
More specifically, the aim of the above mentioned tools is the geometrical description of the regions that have functional role for the proteins that are being studied. The open source application Fpocket and the algorithm Caver, process the input molecular structure, that the user specifies, for potential binding sites. These regions are characterized by their ability to attract other molecules that their function is to work as inhibitors or activators, related to protein functionality. Additionally, the application Caver performs the search in the protein structure for pathways that have their starting point inside the protein molecule and they are directed to the bulk solvent.
Also, in this project the identification of those features that can be used for the prediction of the various regions of interest and have the ability to describe their properties, is being studied. This is performed by the use of machine learning approaches and related feature selection methods.
For the testing of the selected algorithms, a manually curated data set of 260 protein complexes in total was used. A second data set, composed of native protein structures was used in order to test the prediction accuracy of the selected algorithms.

Examining Committee

Phd. Yannis Emiris, Professor - National and Kapodistrian University of Athens (thesis advisor)

Phd. Chrysina Evangelia, Scientific Personnel of IOPC - National Hellenic Research Foundation (NHRF) (thesis advisor)

Phd. Elias S. Manolakos, Assoc. Professor - National and Kapodistrian University of Athens