Pakistan Institute of Engineering and Applied Sciences

Nilore, Islamabad, 45650 Pakistan

THESIS PROJECT PROPOSAL PROFORMA
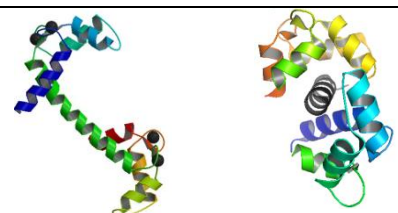
Project Title	**Models for binding associated conformation changes in proteins**
Nature	Computational
Prerequisites	Knowledge of the following will be helpful: • Machine Learning / Computational Intelligence / Pattern Classification / Data mining • Python Programming • Bioinformatics Interested students will be required to take Machine Learning and Bioinformatics (or equivalent) courses if they have not already done so.
Field	Scientific Computing and Computational Intelligence
Expected Cost (if any)	
Work Place*	PIEAS

*define %age of work to be done in PIEAS or at some other place

Supervisor Information

Name of supervisor and designation	Dr. Fayyaz ul Amir Afsar Minhas, Senior Scientist		
Department\Division and Organization	Department of Computer Science, PIEAS		
Contact	Office: 3164	Mobile:	Fax:
Email address	fayyazafsar@gmail.com, afsar@pieas.edu.pk		

Project Details

Synopsis	**Motivation:** Protein molecules are very versatile and dynamic. Some of these molecules can significantly change their structure as a consequence of interacting or binding with other proteins. For example the figures on the right shows the same protein, called Calmodulin, before (left) and after (right) its binding to another protein. Such binding associated conformational changes have great implications in biological processes and require computational modeling and prediction for their understanding. **Objectives:** The objective of this project is to develop machine learning models for identifying binding associated conformational changes in proteins. The model will be given a protein sequence or structure as input. The model's output is a score reflecting the tendency of the proteins to undergo conformational changes. Such a computational model can provide answers for number of biologically interesting questions. **Skills Resulting from the project:** Machine learning, Bioinformatics, Python, Structural Proteomics & Interactomics, Multidisciplinary Research methodologies and publishing.

Goals of the Project

4th Semester (3 credit hour per week are available)	I. **Development of understanding of proteins and their interactions** II. **Learning to handle protein data on the computer** III. **Understanding the underlying basis of binding associated conformational changes.** IV. **Study of properties of proteins useful in prediction of conformational changes.** V. **Hands-on understanding of machine learning techniques** VI. **Developing a baseline predictor**
5th Semester (12 credit hour per week are available)	I. **Analysis of features and classification schemes** II. **Benchmarking the predictor** III. **Development of a webserver for the prediction**

Instructions

- All the columns of project proposal forms are mandatory to be filled.
- The minimum qualification for a supervisor is eighteen years of education plus two years service.
- The minimum requirement for a co-supervisor is eighteen years of education.
- In case of external supervisor (outside DCIS), a co-supervisor will be mandatory from faculty.
- Wherever the project work is carried out (including classified establishments), the defense (only examiners and supervisor) and final presentation (open to all) will be held at PIEAS. The presence of supervisor is necessary for all presentations of fourth and fifth semesters.
- DCIS has right to reject or accept any project.

Signature of Supervisor

Signature Head of the Department
   (With name and designation)