



Project Proposal for Ph.D.

Project Details

Project Title	Determining the Bioactivity information of organic compounds: Development of an experimentally validated reliable computational methodology
Project Summary (Minimum 500 and maximum 2000 characters)	Organic chemists have been synthesizing millions of compounds with novel scaffolds over the decades. Zinc small molecule database boasts of 100 million readily purchasable compounds to help in drug discovery. This despite, number of FDA approved drugs over the last 80 years is just over 2500. In the wake of mounting diseases and new viral and bacterial infections, growing resistance to existing drugs and drying pipeline of drug discovery, it is essential that some novel experimentally validated reliable computational tools be developed to rapidly screen the millions of compounds being synthesized against protein targets for specific diseases. The project involves an understanding of the computational drug discovery protocols, drug-like organic compound scaffolds and their synthesizability and biology of diseases and disorders, assaying protein-ligand binding <i>in vitro</i> and suggestion of lead compounds. Building on the earlier research work carried out in the SCFBIO lab. of IITD, the candidate is expected to evolve a reliable computational tool as a downloadable stand-alone suite and also as a user-friendly web-server for global usage, and validate with real life molecules and <i>in vitro</i> biological assays.

Ph.D. Supervisors

Role	Faculty	Academic Unit in IITD/Institute/University	Email ID (Official)
Supervisor 1	Prof. Vivek Perumal	Kusuma School of Biological Sciences	vperumal@bioschool.iitd.ac.in
Supervisor 2	Prof. Ramu Yadav	Department of Chemistry	Muntha.Ramu.Yadav@chemistry.iitd.ac.in

Project requirements (Student qualifications, experience required, etc)

- The candidate is expected to have Master's degree in Chemistry/Biology/Bioinformatics.
- Also, the candidate is expected to have a sound knowledge of computer aided drug discovery, docking, scoring and molecular simulations in particular.
- The candidate also must have the ability to develop softwares and web-servers for drug discovery.

Source of fellowship/funding

(CSIR/UGC/DBT/ICMR/ICAR/NEET-PG/DST-INSPIRE/IRD/FITT Project details, if any)

DBT Project of IRD (RP04062G)

Role of Faculty Members involved:

Prof. RY will supervise work on the chemistry of organic compounds, synthesizability of drug-like scaffolds and their modifications for improved target binding.

Prof. VP will supervise work on the biology of diseases, druggable protein targets, protein-organic molecule binding assays etc..

Prof. BJ will supervise work on computational tools for scanning organic compounds against protein targets.