



Project Proposal for Ph.D.

Form Approved by SIRe

Project Details (The research problem must clearly indicate the need for an interdisciplinary approach)

Project Title	Development of Quantum Computing based Pipeline for Computer Aided Drug Design
Project Summary (Minimum 500 and maximum 2000 characters)	Computational tools are central to drug discovery, yet classical methods struggle with the exponential scaling of biomolecular simulations. Quantum algorithms such as the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) have already been applied to small molecules (e.g., H₂, LiH, BeH₂), showing that quantum devices can capture electronic states beyond classical Density Functional Theory (DFT). Recent IBM and Google demonstrations highlight the promise of hybrid quantum classical approaches, yet systematic adaptation of classical methods to quantum platforms remains limited. This project proposes a quantum computer aided drug design (QCADD) pipeline that integrates quantum molecular simulation with quantum-enhanced screening, coupled with experimental guidance to accelerate and improve drug discovery. Objectives We hypothesize that quantum computing will enhance small-molecule screening and accelerate the identification of drug-like candidates. Specifically, QCADD aims to: (i) replace traditional drug-likeness rules with quantum state based molecular descriptors for more reliable filtering, (ii) improve docking accuracy through quantum methods such as QPE to refine binding energies, (iii) adapt established classical pipelines (e.g., Sanjeevini/Dhanvantari) to quantum platforms as proof-of-concept, and (iv) develop hybrid workflows that demonstrate measurable advantages over conventional HPC methods. To ensure practical relevance, QCADD will be coupled with experimental validation. Predicted drug-likeness of small molecules will be tested using biophysical and biochemical assays, with feedback refining algorithms, benchmarking accuracy, and improving performance. This interdisciplinary project, co-led by Prof. Tarak Karmakar (Chemistry, quantum algorithms and molecular modeling) and Prof. Ashok Patel (Biological Sciences, structural biology and assays), integrates quantum computation with experimental biology to deliver a translational platform for next-generation drug discovery.

Ph.D. Supervisors*
(Supervisor 1 and Supervisor 2 cannot be from the same department of IITD)

Role	Name of Faculty	Academic Unit in IITD/Institute/University	Email ID (Official)
Supervisor 1*	Prof Ashok Kumar Patel	Kusuma school of Biological Sciences	ashokpatel@bioschool.iitd.ac.in
Supervisor 2	Prof Tarak Karmakar	Chemistry	tkarmakar@iitd.ac.in

*Supervisor 1 must be from IIT, Delhi.
+All cells in this table are mandatory fields that need to be filled by faculty for consideration of proposal.
§The date of superannuation of supervisors should be at least three years from the date of registration of selected candidates.

Project requirements (Student qualifications, experience required, etc)
*The candidate will be shortlisted based on common shortlisting criteria decided by ScRC (SIRe)

- Candidate is required to have M.Sc. in chemistry with desertion project in computational chemistry. Further, understanding of docking, molecular simulation etc., is bonus.
- Programming in Python is desirable with the basic understanding of Linux and bash scripting.

Source of fellowship/funding and project number

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

Candidate with his/her own fellowship.

Role of Faculty Members involved:

Supervisor-1

Guide biophysical and biochemical assays for the experimental validation of QCADD pipeline.

Supervisor-2

Guide designing the computational workflow of QCADD pipeline through his expertise in computational chemistry, quantum algorithms, and molecular modeling.

Note :-

1. **Approval from the respective DRC/CRC/ScRC of your Department/Centre/School will be required for using the "Full-time Institute Assistantship (Category-wise) (FIA)" for selecting the students in SRe.**
2. **Declaration:- Faculty members, please ensure that you have at least 3 years of service left before superannuation along with adequate sitting space & lab facilities for the SRe student.**
3. **PI/s are also encouraged to submit joint proposals with AIIMS, NII, JNU and institutes with which IITD has an existing MoU. If the Co-PI (Supervisor 2) is from outside IITD, kindly share his/her detailed CV.**
4. **If a research scholar is to be considered for selection under the project fellowship, then the project should have a minimum of two-year duration remaining.**
5. **A candidate applying with a valid JRF/INSPIRE/any national level fellowship should have at least two-year validity from the date of joining the Ph.D. program.**
6. **The third supervisor’s name (if required) can be added only after the formation of Student Research Committee (SRC) subject to a strong recommendation of SRC and subsequent approval from the competent authority.**
7. **If Institute fellowship is being sought, then DRC approval of the parent department of Supervisor 1 is required at the time of selection.**