





HIGHLIGHTS OF THE COURSE

- PROTEIN CRYSTALLIZATION AND STRUCTURE SOLUTION
- PROTEIN STRUCTURE, FUNCTION, BIOINFORMATICS & INHIBITORS.
- IDENTIFICATION OF KEY DRUG TARGETS IN LIFE THREATENING DISEASES
- UNDERSTANDING THE DATABASES IN PROTEIN RESEARCH
- MOLECULAR MODELLING -HOMOLOGY AND AB INITIO MODELING
- STRUCTURE BASED DRUG DESIGNING

TRAINING IN COMPUTATIONAL AND STRUCTURAL BIOLOGY

The revolutions in the proteomics and structural genomics has solved the structures of several macromolecules. These structural information often enables life-science researchers to address a wide variety of research questions. The structural data not only helps in the elucidation of molecular interactions but also aids in the understanding of mechanistic effects of single nucleotide polymorphisms that are having disease relevence. The structural data plays an important role in structure based drug design by proposing the key interactions of drug molecules. It also helps in predicting the protein-protein and protein-nulceic acid interactions that are a part of complex biological network.

We at Jubilee Centre for Medical Research is providing a **six months foundation course** in computational and structural biology. The course is meant for the biological researchers who wish to learn more about the macromolecular structures, how these structures are solved and how to use key bioinformatics resources for the computational and structural biology. No previous experience in the field of structural bioinformatics is required, however a basic knowledge of protein structure would be of benefit. For more information, contact us.

Course Coordinator: <u>Dr Dileep Vijayan</u> <u>Laboratory for Computational and Structural Biology</u>

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JUBILEE CENTRE FOR MEDICAL RESEARCH

Training in Computational and structural Biology

PROGRAM SPECIFIC OUTCOMES:

Upon completion of the programme, the candidate is expected to gain the following attributes:

- Technical skills and hands on experiences in bioinformatics, computer aided drug design, structure based drug design, molecular modeling, protein crystallization, *in vitro* drug-ligand interactions, X-ray crystallography etc.
- Confidence in the research career and critical thinking ability to review scientific literature as steppingstone to research.
- Ability to work independently in chosen research topics as well as be part of teamwork with collaborative skills and become future scientists, teachers, and entrepreneurs in the area of computational and structure biology.

ELIGIBILITY FOR ADMISSION:

Student with bachelor's or master's degree in any branch of science/technology/medicine.Eligible subject areas include: Life sciences (botany, zoology, genetics, human biology, general life sciences, ecology, environmental biology), bioinformatics, microbiology, biotechnology, chemistry, physics, mathematics, computer science/information technology, statistics, any branch of engineering, pharmaceutical sciences, agriculture, medicine, dentistry, horticulture, forestry, and veterinary sciences.

DURATION AND OTHER DETAILS OF THE PROGRAMME:

Course Duration: 6 Months.

Number of intakes: 3 candidates.

Syllabus:

Module 1: Introduction to databases – Primary, secondary and composite databases. Overview of types of biological data: Sequence and structure data. Overview of GenBank, EMBL, DDBJ, Swiss-Prot, UniProt, MMDB, SCOP, CATH, KEGG ENZYME, BRENDA, Prosite, ProDom, Pfam, PDB etc.

Module 2: Biomolecular simulations – Molecular Visualization, Structure preparation for computational experiments, Energy minimization, MD simulations, analysing trajectory, structure based drug design, molecular docking, scaffold hoping etc.

Module 3: Protein structure solution – Protein structure prediction, homology modeling, ab initio modeling.

Module 4: Protein crystallography – crystallization, handling protein crystals, protein structure solution, handling crystallographic data.

Module 5: Key details of scientific writing – Research design, data collection and analysis, reporting research results. Structure of different kinds of scientific papers, steps in the publication process, IMRAD, journal impact factor, selection of appropriate journals, explanation on predatory journal, scientific misconduct. Figure generation.

