

Bioinformatics Infrastructure Facility, Jamia Hamdard **Hamdard Nagar, New Delhi 110062**

Facilities & Activities

Bioinformatics Infrastructure Facility (BIF) at Jamia Hamdard was created in 2008-09 under the BTBI program of DBT, Ministry of Science and Technology with the objective of supporting bioinformatics training and research in the University in life, pharmaceutical and medical sciences.

Areas of specialization:

The center has identified drug design, protein structure prediction, computational biochemistry, and systems biology as thrust areas for research in bioinformatics, besides providing training in the identified areas through seminars and by other means.

Major activities:

BIF is the center for bioinformatics studies at Jamia Hamdard, supporting ongoing teaching and research activities of the University in bioinformatics. The center is also engaged in providing support to researchers from outside the university, and makes its infrastructure available on request. University has recently started PhD programs in Bioinformatics and in Chemoinformatics. The center is working in collaboration with other institutes such as URDIP (CSIR) (Pune), ICGEB (New Delhi), and IIIM (Jammu), with whom the University has signed MoUs. Besides the University faculty, the Board of Research Studies has recognized some senior scientists of these institutes with orientation in bioinformatics to act as Supervisors/Co-supervisors of students registered for PhD Bioinformatics and PhD Chemoinformatics. The PhD program in bioinformatics is under the Faculty of Engineering and Interdisciplinary Sciences of the University.

Research at BIF Jamia Hamdard is currently focused on protein, its tertiary structure prediction and role in signaling, besides continuing the work on computational design of some novel, non-pteridine analogs as selective *Mycobacterium tuberculosis* dihydrofolate reductase inhibitors. Designing and development of new anti-malarial agents by generating a robust QSAR model of novel synthetic agents is another area of current research. In the area of computational protein structure prediction, center is working on some peptides isolated from scorpion, and has predicted the tertiary structure of a couple of peptides using bioinformatics tool. Earlier, in 2009, center carried out studies on prokaryotic and eukaryotic non-membrane proteins, and published a paper in the Journal of Computer Science and Systems Biology 2(6), 298-299. Understanding the role of osmotin, an osmoregulatory protein in plant, in cell signaling under stress using protein modeling and docking tools is another area where the center is involved.

The BIF JH has been organizing a series of seminars-cum-hands-on training programs in bioinformatics. First seminar in the series was organized in 2009 on Bioinformatics Applications in

Computer Aided Drug Design to familiarize and sensitize the participants the practical applications of computational chemistry in drug discovery, visualizing the intermolecular interaction networks in protein-ligand complexes, modeling and docking to flexible receptors, QSAR/QSPR, virtual screening and computer-aided design and optimization. In 2010, second seminar-cum-hands-on training was organized on Chemo-bioinformatics and Computational Biology to familiarize the participants with e-pharmacophore, superdrug database, GPCR structure modeling, and SciFinder. Eminent researchers, academicians and representatives from industry were invited. The third seminar in the series was on Computational Protein Structure Prediction, and organized in November 2011. This seminar provided an opportunity to the participants from various disciplines to learn computational methods of prediction of protein structure. Scope of the seminar was much broader than critical assessment of homology modeling, and focused more on the analysis of results, and validation process. Participants were given hands-on training on construction of atomic resolution model of the target protein from its amino acid sequence using an experimental 3-D structure of a related protein as template using Swiss model assessment server, FASTA, BLAST, and some licensed software through guided practical training by experts.

Infrastructure:

BIF is equipped with a dedicated high-end Database/Application server and a medium-end Proxy & File server, Desktops (11) with OS, and license for molecular modeling software (vLife MDS 3.5), which is also made available to users outside the University on request. Center is in the process of updating its infrastructure, and trying to procure licensed software for studies on protein.

Manpower:

Presently the facility is looked after by a team comprising of the following:

1. Prof. Shakir Ali, *Coordinator, BIF*
Head, Department of Biochemistry &
In-charge, Faculty of Engineering and Interdisciplinary Sciences
2. Dr. Mymoona Akhtar, *Dy. Coordinator, BIF*
Asstt. Prof., Pharmaceutical Chemistry

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