**RESEARCH PROFILE**

The broad research area includes Computer Aided Drug Design, Systems Biology, Structural Biology and Pharmaceutical Sciences.

My Specific area of research includes Molecular modeling, drug design strategies and Molecular dynamics Simulation for G-Protein Coupled receptors (GPCRs) including both computational and experimental approaches.

**Brief Outline**

The ability to design drugs effectively depends on the fundamental understanding of the structures of molecules and the biochemical interaction networks. The past decade has witnessed a paradigm shift in drug discovery with structure-based drug design playing a crucial role. The gap between the number of identified hits and actual drug candidates can be bridged by investigating the underlying interactions. A pool of information combining crystallographic structures and molecular modeling techniques permits to predict receptor 3D models of good quality. These models serve as a basis to establish and validate efficient rationales used to screen virtual libraries for obtaining hits. An integrated approach combining structure based drug design, systems biology and biological circuits can help in gaining synergy in drug design.

The role of these approaches with respect to two different classes of pharmaceutical targets is being studied.: (a) *Plasmodium falciparum* metalloaminopeptidases, promising targets for anti-malarial drug development. It regulates the intracellular pool of amino acids required for the growth and development of malarial parasite. (b) G-protein coupled receptor- particularly orphan GPCRs reported to be predominantly expressed in pancreatic β –cells and a plausible target for treatment of type 2 diabetes mellitus.

The methodology employed includes Gene analysis, structure prediction of proteins, Molecular mechanics and molecular dynamics simulations, structure based drug design strategies, system biology approaches and designing of biological circuits. The results are validated further by pharmacological and biological assays.

**Eminent Scientists Working in the Area**

1. **Prof Thomas T Cheatham**

Director, Research Computing / Center for High Performance Computing

University Information Technology, University of Utah

USA

1. **Prof. B.Jayaram**

Professor, Department of Chemistry & School of Biological Sciences,

Coordinator Supercomputing Facility for Bioinformatics & Computational Biology

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