## Methods and techniques in integrated Structural Biology: Toward structure based drug development

#### Overview

Structural biology has witnessed much rapid advancements in recent years. Modern advancements in the structure determination techniques of macromolecular assemblies: X-ray crystallography and cryo-electron microscopy have made it possible to obtain three-dimensional structural information on various biological processes and systems with much less effort than in the past. The availability of atomic resolution structures provides a deep and unique understanding of protein function, and helps to unravel the biological chemistry of biomolecules. Using the three-dimensional structure of biological macromolecules to infer how they function, is one of the most important fields of modern biology. Over the past few decades, the appreciation and realization that the 3D structures of proteins have the potential to accelerate the drug discovery process. Additionally, structure based rational drug designing has radically transformed due to advances in genome sequencing, robotics and bioinformatics. The science of structure determination and structure based drug discovery has taken a rapid advancement and owes much of it to the sideways development of computer-controlled diffractometers for routine data collection, high speed computers for data analyses and powerful computer graphics, which allows real-time visualization and manipulation of atoms and functional groups of lead drug molecules against a specific drug target.

The integration of structural biology using different techniques will help to understand the basis of detailed atomic structure, how proteins, protein complexes or whole pathogens interact dynamically with their functional environment. This requires substantial knowledge in the field of X-ray crystallography, cryo-electron microscopy and computational biology, and helps us to see in atomic detail the mechanisms by which healthy cells function and diseases progress. This fundamental understanding will underpin our ability to provide new therapeutics to meet the grand challenges in human health.

The primary objectives of the course are as follows:

- i) Exposing participants to the fundamentals of structural biology methods,
- ii) Understanding various techniques of integrated structural biology
- iii) Building confidence and capability amongst the participants in the application of structural biology, i.e. structure based drug development and protein engineering
- iv) Providing exposure to practical problems and their solutions, through case studies and understanding of fundamental biological processes as well as numerous applications to improve human health

Course participants will learn these topics through lectures and hands-on experiments. Also case studies and assignments will be shared to stimulate research motivation of participants.

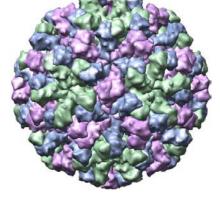
Course	Methods and techniques in integrated Structural Biology: 15 <sup>th</sup> – 21 <sup>st</sup> Jan, 2018	
	Number of participants for the course will be limited to fifty.	
You Should Attend If	<ul> <li>Executives, engineers and researchers from manufacturing, service and government organizations including R&amp;D laboratories.</li> <li>Student at all levels (B. Tech. / M. Sc. / M. Tech. / Ph. D.) or Faculty from reputed</li> </ul>	
	academic institutions and technical institutions.	
Fees	The participation fees for taking the course is as follows:  Participants from abroad: US \$500  Industry/ Pvt. Research Organizations: Rs. 10,000/-	
	Academic Institutions: Rs. 3000/- (for faculty), Rs. 2500/- (for post-docs), Rs. 1000/- (for B.Tech. and M.Sc. students) and Rs. 2000/- (for Ph.D. students)	
	For Registration: Registration form is attached below	
	The above fee includes all instructional materials, computer use for tutorials, 24 hrs free internet facility.	
	The participants have to bear the food and lodging expenses during their stay. The participants will be provided with single bedded accommodation on Twin sharing basis/single occupancy on payment basis.	

### The Faculty



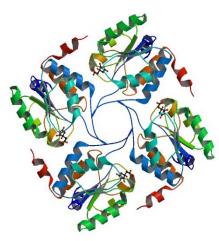
**Prof. BVV Prasad** is Alvin Romansky Chair in Biochemistry, Baylor College of Medicine, Houston, Texas, United States. His work is focused on structure-function relationships in medically important viruses with a clear emphasis on using the knowledge to develop/design effective antiviral drugs. The fascinating

aspects of his study are the virus replication process and how these viruses counteract the antiviral response mounted by the host cells, for example, interferon response. Each virus appears to specially designate a viral protein to antagonize the host immune response. In rotavirus, it is the non-structural protein NSP1 and in influenza virus it is NS1. During this process, these viral proteins target critical cellular pathways by interacting with various cellular proteins.





**Dr. Pravindra Kumar** is Associate Professor in Department of Biotechnology, IIT Roorkee. He uses X-ray crystallography as the major tool for investigating the structure and function of enzymes and seeks to enhance their functional capabilities, to manipulate their activities, and to design and develop functional therapeutic agents.





**Dr. Saugata Hazra** is Assistant Professor in Department of Biotechnology, IIT Roorkee. He works in the field of protein crystallography; structure based drug development and computational biology, MD simulation, Virtual screening and Macromolecular interaction.

#### Course Co-ordinator

**Dr. Pravindra Kumar** 

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http://www.gian.iitkgp.ac.in/GREGN

# GIAN Course on "Methods and techniques in integrated Structural Biology: Toward structure based drug development" @ IIT Roorkee 15<sup>th</sup> to 21<sup>st</sup> Jan. 2018

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