

# Chemical Biology and Drug Discovery

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## Overview

Chemical biology is the application of chemical tools and ideas to probe biological systems and solve medical problems. The approach is highly interdisciplinary and involves the interaction of, for example, chemists with biochemist, enzymologists, cell biologist and/or protein scientists etc. With comprehensive introduction to the origins and emerging frontiers of chemical biology, this course will develop the fundamental chemistry of molecules found in nature and help in understanding (i) What is chemical biology?; (ii) How can chemistry be used to advance the study of biological systems? and (iii) How knowledge of chemical biology is important for the discovery of new drugs and advance science and human health? Technological advances have allowed chemical biologist to employ both large libraries of small molecules and robust screens for biological activity to decipher complex biological systems. This approach benefits from both a grasp of basic synthetic chemistry and an understanding of molecular biology, representing a true intersection of the two fields. The goal of the course is to familiarize students with innovative recent experimental approaches and to stimulate them to conceive their own new ideas/methods to advance biomedical research.

## Objectives

The primary objectives of the course are i) to educate the participants to read, interpret and present primary literature in the field of chemical biology and apply to develop a testable question or hypothesis stemming from previous work in the field of chemical biology, ii) to introduce experimental skills used in chemical biology such as protein purification, biopolymer synthesis and purification, microscopy, protein-ligand characterization, protein/peptide mass spectrometry, iii) to teach about chemical biology approaches to drug discovery and development by specifically targeting proteins and introduce various chemical biology techniques and applications and iv) to give an overview of medicinal chemistry and drug discovery process at the Pharma Industry and at few leading institutes in India and in USA.

<b>Modules</b>	<b>Module A:</b> Introduction to chemical biology and drug discovery <b>Module B:</b> Use of small molecule probes to unravel cell biology <b>Module C:</b> Understanding the molecular biology and recent experimental tools <b>Module D:</b> Case studies to give an overview of drug discovery process at the Pharma Industry and at few leading institutes in India and in USA. October 24 - October 30, 2017 Number of participants for the course will be limited to fifty.
<b>Who Should Attend ?</b>	<ul style="list-style-type: none"><li>▪ Executives, engineers and researchers from manufacturing, service and government organizations including R&amp;D laboratories.</li><li>▪ Students at all levels (BTech/MSc/MTech/PhD) or faculty from academic institutions and technical institutions interested in learning about "Chemical Biology &amp; Drug Discovery"</li></ul>
<b>Fees</b>	The participation fees for taking the course is as follows: <b>Participants from abroad : US \$300; Participants from Industry: INR 5000;</b> <b>Faculty and Research Scholars from University, Institutes and Colleges: INR 2500;</b> <b>Bachelors and Masters Degree students: INR 1500</b> The above fee includes all instructional materials and assignments and 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

## The Faculty



**Prof. Sanjay Malhotra** is a faculty in the Department of Radiation Oncology, Radiology and Stanford Cancer Institute at the Stanford University School of Medicine. He is also a Director of Stanford-SRI Drug Discovery and Development Program. He has over 20 years of experience in basic and translational research in biomedical

sciences. His efforts have led to advancement of several drug candidates towards their pre-clinical studies and clinical trials. Dr. Malhotra has edited five books, published over 100 research articles and serves on the editorial board of international scientific journals. He has received numerous honors including, 'Fulbright Specialist' (US); Fellow Royal Society of Chemistry (UK); 'Invited member' INDO-US Science & Technology Joint Commission Meeting, Office of the Science & Technology Policy of the President (White House). Dr. Malhotra received a PhD (Chemistry) in 1995 and trained under Nobel laureate Prof. Herbert C. Brown at Purdue University.



**Dr. Deepak Salunke** received his PhD at Organic Chemistry Division of CSIR-National Chemical Laboratory (NCL), Pune with Dr. Vandana Pore and Dr. Braja Gopal Hazra, and worked on the Medicinal Chemistry of steroidal conjugates. He also worked on a Indo-French Sandwich Thesis program at ICSN-CNRS France with Dr. Robert H. Dodd.

After his PhD, he worked at the Advinus Therapeutics Pvt. Ltd. in a discovery working group towards the development of GPR91 antagonists. Later he moved to NCTU Taiwan to work at the combinatorial chemistry laboratory of Prof. Chung-Ming Sun. After spending one year at NCTU, Dr. Salunke moved to Department of Medicinal Chemistry at the University of Kansas (KU), Lawrence, USA and then promoted as Assistant Research Professor at Higuchi Biosciences Centre at KU. Before joining at the Panjab University, Chandigarh he worked as a Team Leader at the SAI Life Sciences Pvt. Ltd. Pune. Dr. Deepak Salunke is engaged in research involving design, synthesis and Structure-Activity Relationships (SAR) of novel pharmaceutically interesting scaffolds. Combinatorial parallel synthesis as well as diversity-oriented synthesis of organic small molecules and to develop innovative methodologies for important organic transformations. He has recently been awarded a travel grant by NCTU to deliver a lecture series at Taiwan and also delivered several invited talks at National and International conferences.

## Course Co-ordinator

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

## Course Outline

- Day-1**
1. What is chemical biology
    - Historical and Philosophical aspects
    - Bringing chemical solutions to biological problems
  2. Chemical biology and drug discovery
    - Understanding biological space
  3. Chemical biology and drug discovery
    - Exploring chemical space
- Day-2**
4. How to unravel biological mechanism
    - Use of Small molecule probes
    - Using natural products to unravel cell biology
  5. Controlling protein functions
    - Small caged molecules to control protein activity
  6. Controlling protein functions
    - Resistance mutations and small molecule agents
  7. General introduction to Medicinal Chemistry
- Day-3**
8. Protein-Protein Interactions
    - Using chemical induces and disruptors of dimerization
  9. Protein-Protein Interactions
    - Protein secondary structure mimetics as modulators of PPI and
    - Protein-ligand interactions
  10. Protein-Ligand Interactions
    - Role of ligand-dependent transcription regulators
  11. HIT Identification
- Day-4**
12. Forward Chemical Genetics
    - Small molecules for perturbing biological systems
  13. Reverse Chemical Genetics
    - Study of protein function for drug discovery
  14. Chemical biology and Enzymology
    - Protein phosphorylation (case study)
  15. Lead Identification
- Day-5**
16. Chemical Strategies for activity based proteomics
    - Introduction and case study
  17. Tags and Probes for chemical biology
    - Introduction and case study
  18. Chemical Informatics
    - Computational methods and modeling
  19. A case study on the Discovery of GPR antagonist
- Day-6**
20. An overview of Drug Discovery Working Group at Indian Biotech companies
  21. Current trend of research at Indian Contract Research Organizations
  22. Drug discovery approaches at the University/Institutes: A comparison between Indian and US approach.