Overview of the Course

Cancer and viral infections remain a fundamental burden to public health despite substantial efforts aimed at developing effective drug therapies. The design and optimization of anti-cancer and anti-viral drugs is a difficult task. Among the many challenges involved are the selective targeting of bio macromolecules and emerging drug resistance. Today, bioinformatics and cheminformatics methods are key components of any drug discovery and development pipelines, and highly successful in addressing these problems effectively.

This course will teach the skills and knowledge required for the design and optimization of anti-cancer and anti-viral drugs using computer-based methods. Topics include concepts for model validation and the latest methods for drug ability prediction, for polypharmacology and the assessment and optimization of ADME properties. Finally, all participants will summarize and present their findings in form of a short talk in the presence of all fellow participants, where they point out their strategies of finding anti-cancer and anti-viral compounds, and motivate their selection of candidate molecules.

Course Contents:

The main objective of the proposed course is to provide Overview of the latest concepts and methods in the computer-based anti-cancer and anti-viral drug discovery, Overview of the most promising anti-cancer and anti-viral targets, key data resources and software. Knowledge of the most relevant ligand-based and structure-based approaches for the identification, design and optimization of anti-cancer and anti-viral compounds. Ability to assess the quality of data and models. Ability to independently and effectively apply state of the art methods in Bioinformatics and Cheminformatics to identify, design and optimize anti-cancer and anti-viral compounds.

Prof. Johannes Kirchmair is Professor of Applied Bioinformatics at University of Hamburg, and Head of the Research Group for Applied Cheminformatics and Molecular Design. He worked as a research associate at the Centre for Molecular Informatics, University of Cambridge, and was leading a research project on drug metabolism prediction at ETH Zurich. His main research interests include the development and application of computational methods for the prediction of the bioactivity and metabolism of xenobiotics (drugs and drug-like molecules, cosmetics, agrochemicals and functional foods). For more details: http://www.zbh.uni-hamburg.de/en/johannes-kirchmair-prof-dr.html

Dr. Raju Bhukya received Ph.D. degree in Computer Science and engineering from the National Institute of Technology Warangal, Telangana State (India). Currently he is working as an Assistant Professor at the same institute since 2006. He has published several papers in international journals and conferences. His research areas include Bioinformatics, DNA data optimization, DNA Data Compression, Molecular Data Analysis, Pattern matching .

Who can Participate?

This program is open to the Faculty, PG and Research students of Computer Science and Engineering, Bioinformatics, Biotechnology, Pharmacy, Chemical, Chemistry and other relevant streams from various institutes. Candidates from industries, research labs can also participate.

How to Register?

Stage-1: Web Portal Registration:Visit http://www.gian.iitkgp.ac.in/GREGN/index and create login User ID and Password. Fill up the blank registration form and do web registration by paying Rs. 500/- online through Net Banking/Debit/Credit card. This provides the user with life time registration to enroll in any number of GIAN courses offered.

Stage-2: Course Registration:

Login to the GIAN portal with the user ID and Password already created in Step 1. Click on Course Registration option at the top of Registration form. Select the Course titled "**Computer–Based Methods for Anti-Cancer and Anti-Viral Drug Discovery**" from the list and click on Save option. Confirm your registration by clicking on Confirm Course.

Registration Fee:

Faculty	Rs. 4,000/-
Participants from Industry /Research Organizations	Rs. 10,000/-
Students & Research Without award of Grade With award of Grade	 Rs. 1,000/- Rs. 2,000/-
Students from abroad	$ 300

The Registration fee includes instructional materials, tutorials, laboratory and computer use and free internet facility. The participants from academic/research institutes and Industry will be provided with boarding and lodging on additional payment of Rs. 4,000/- in Visitors Block on sharing basis. Students & Research Scholars will be provided with boarding and lodging in Institute Hostels on additional payment of Rs. 2,000/-.

Selection and Mode of Payment

Selected candidates will be intimated through e-mail. They have to remit the necessary course fee to the Bank as per the details given below.

Outstation participants requiring accommodation and boarding facilities have to pay Rs. 4,000/- in addition to the course fee.

Accout Name	GIAN NITW
Account No.	62447453600
Bank	State Bank of Hyderabad
Branch	REC Warangal (NIT Campus)
Branch Code	20149
IFSC	SBHY0020149
MICR Code	506004011
SWIFT Code	SBHYINBB018

Candidates registering early will be given preference in short listing process

For any queries regarding registration of the course, please contact the National Coordinator:

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National Institute of Technology
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About GIAN Course

MHRD, Govt. of India has launched an innovative program titled "Global Initiative of Academic Networks (GIAN)" in higher Education, in order to garner the best international experience. As part of this, internationally renowned Academicians and Scientists are invited to augment the Country's academic resources, accelerate the pace of quality reforms and elevate India's scientific and technological capacity to global excellence.

About the Institute and Warangal

National Institute of Technology, Warangal (NITW) formerly known as RECW is the first among seventeen RECs set up in 1959. Over the years, the Institute has established itself as a premier Institution in imparting technical education of a very high standard, leading to B.Tech, M.Tech and Ph.D. programmes in various specializations of Science and Engineering streams. Warangal is known for its rich historical and cultural heritage. It is situated at a distance of 140 km from Hyderabad. Warangal is well connected by rail and road. National Institute of Technology, Warangal campus is 2 km away from Kazipet railway station and 12 km away from Warangal railway station.

About the Department

The Department of Computer Science and Engineering (CSE) offers B.Tech course in CSE, M.Tech courses in CSE, Information Security (IS) and Master of Computer Applications (MCA). The Department has experienced faculty with good publications and well-established laboratories. The Department has liaison with reputed industries and R&D organizations like Microsoft, IBM, Oracle, Accenture, Infosys, TCS, EMC2, C-DAC, Motorola, NIC, Sun Micro Systems, SPSS and tie up with IISc in certain areas.

A Ten Day

GIAN Course

on

Computer-Based Methods for Anti-Cancer and Anti-Viral Drug Discovery

December 10 - 19, 2016

Call for Registration and Participation

Resource Person

Prof. Johannes Kirchmair

Applied Bioinformatics
University of Hamburg

National Coordinator
Dr. Raju Bhukya

Department of Computer Science & Engineering
National Institute of Technology
Warangal – 506 004, Telangana
India

Workshop Tentative Topics	
Day 01	Chapter 1: Introduction: Design and optimisation of anti-cancer and anti-viral compounds
	Chapter 2: Evolution of experimental approaches and design strategies
	Chapter 3: Computer-based approaches for design and optimisation of anti-cancer and anti-viral compounds
Day 02	Chapter 4: Data sources
	Chapter 5: In silico description of small molecules
	Chapter 6: Empirical force fields and conformational search
Day 03	Chapter 7: Ligand-protein interactions exemplified with relevant drug targets
	Chapter 8: Chemical similarity
	Chapter 9: Use and interpretation of experimental data for in silico modelling
Day 04	Chapter 10: Preparation of chemical data for in silico modelling
	Chapter 11: Structure-activity relationship modelling
	Chapter 12: Analysis and preparation of protein structural data
Day 05	Chapter 13: Ligand-based methods for identification of anti-cancer and anti-viral compounds
	Chapter 14: Structure-based methods for identification of anti-cancer and anti-viral compounds
	Workshop: Working with protein structures relevant to anti-cancer and anti-viral drug design
Day 06	Chapter 16: Validation of in silico models
	Chapter 17: De novo design of anti-cancer and anti-viral drugs
	Workshop: Analysis of protein-ligand interactions
Day 07	Chapter 19: In silico methods for druggability prediction
	Chapter 20: In silico methods for polypharmacology
	Workshop: Development of structure-based models for virtual screening for anti-cancer and anti-viral compounds
Day 08	Chapter 22: In silico prediction of pharmacokinetic parameters
	Chapter 23: Scientific workflow systems for the design and optimisation of anti-cancer and anti-viral compounds
	Workshop: Development of structure-based models for virtual screening for anti-cancer and anti-viral compounds I
Day 09	Workshop: Development of structure-based models for virtual screening for anti-cancer and anti-viral compounds II
	Workshop: Preparation of molecular libraries for virtual screening
	Workshop: Virtual screening for anti-cancer and anti-viral compounds I
Day 10	Workshop: Virtual screening for anti-cancer and anti-viral compounds II
	Workshop: Assessment of the ADME, toxicity and polypharmacology profiles of the hits
	Workshop: Presentation, discussion and conclusion.