



Community of Practice for
Drug Discovery & Development

DRUG DISCOVERY

DESIGN METHODS & APPLICATIONS

January 5–9, 2015,
Institute of Life Sciences,
Ahmedabad University, Ahmedabad, India

Structure-based drug design, cheminformatics, bioinformatics
and molecular modelling supporting drug design & discovery



A hands-on 5 day eCheminfo workshop week with a
case study focus in anti-malarial drug design.

LED BY

ALESSANDRO CONTINI

BARRY HARDY AND ALOK DHAWAN

Work through in detail and discuss case studies,
practical examples, methods and emerging techniques
with leading modelling experts!

PRE-CONFERENCE CRICKET MATCH *AND SOCIAL DINNER*

SUNDAY, JANUARY 4TH 2015

*echeminfo*INDIA



There will be a pre-conference social event including a Cricket match on Sunday January 4th 2015, in the afternoon. The match will be of 10 overs a side and played with Tennis balls. All participants are encouraged to attend this event since it will also give them time to interact and get introduced.

The social dinner will be at a venue outside the ILS campus and is sponsored by the organizers.

Help desk will be available throughout the day for registration, software updates and any other assistance that may be required.



DRUG DISCOVERY 2015

PROGRAM TOPICS

MONDAY, JANUARY 5 TO FRIDAY, JANUARY 9

- ✘ Functional kinomics of Plasmodium-infected erythrocytes
 - ✘ Genome wide functional analysis of Plasmodium kinases and Phosphatases
 - ✘ Homology modelling and loop refinement using Phosphoglycerate kinase
 - ✘ A real world drug discovery study
 - ✘ Structure preparation and docking experiments with SPORES/PLANTS
 - ✘ Docking strategies
 - ✘ Group work and discussion on workshop case study problems
 - ✘ Poster session with refreshments and food
 - ✘ Virtual screening with shape: How well will we do?
 - ✘ MM-PBSA/GBSA free energy of binding calculations on protein kinase Ligands
 - ✘ ADME & Toxicology profiling
 - ✘ Review, further work, experimental testing of predictions
-

Douglas Connect
Working communities



WORKSHOP LEADERS

ALESSANDRO CONTINI

University of Milan

WORKSHOP CO-CHAIR



Professor Alessandro Contini graduated in 1999 with a degree in Chemistry and Pharmaceutical Technologies from the University of Milan. He then spent a period as a visiting scientist in the laboratory of Prof. Leonardo Scapozza, ETH, Zurich, where he learned the basis of molecular modelling, and in 2003 he obtained a Ph.D. in medicinal chemistry (University of Milan).

He continued his studies in molecular modelling, supporting the experimental chemistry units by studying reaction mechanisms and predicting optical and spectroscopic properties of organic molecules with quantum-mechanical techniques.

In 2006 he was appointed Assistant Professor of organic chemistry at the University of Milan, where he teaches organic chemistry in the Faculty of Pharmaceutical Sciences. He started an independent computational chemistry laboratory which hosts undergraduated and graduated students, as well as post-doc fellows, working tightly with experimental chemists and pharmacologists and covering several aspects of molecular modelling, such as computational organic chemistry, drug design, structure activity relationships, pharmacophore modelling, virtual screening, biomolecular interactions, molecular dynamics and conformational analyses of natural and non-natural biomolecules.

Dr. Contini co-authored 45 articles in peer reviewed international journals and several other scientific contributions. Since 2010 he is involved in the Scientists against malaria initiative (SAM) for the identification of kinase inhibitors with antimalarial activity.

BARRY HARDY

Douglas Connect

WORKSHOP CO-CHAIR



Dr. Barry Hardy currently manages the eCheminfo and InnovationWell community of practice activities of Douglas Connect and the training programs of the Knowledge Management Institute, Switzerland.

He obtained his Ph.D. in 1990 from Syracuse University working in the area of computational chemistry, biophysics and computer-aided molecular modelling and drug design.

Dr. Hardy has also been working in the area of knowledge management and communications since 1994 and has organised numerous international projects in the area of the chemical, life and medical sciences.

He has also developed technology solutions for internet-based conferencing, tutor-supported e-learning, laboratory automation systems and computational chemistry and informatics. He is currently leading the Application and Knowledge Assessment Activities for the SYNERGY FP7 ICT project on Knowledge-oriented Collaboration, and serving as Coordinator for the OpenTox FP7 Health project on Predictive Toxicology.

Dr. Hardy was a National Research Fellow at the FDA Center for Biologics and Evaluation, a Hitchings-Elion Fellow at Oxford University and CEO of Virtual Environments International.

ALOK DHAWAN

Institute of Life Sciences

WORKSHOP CO-CHAIR



Professor Alok Dhawan, Director, Institute of Life Sciences, Ahmedabad University, Gujarat, on lien from CSIR-Indian Institute of Toxicology Research, Lucknow where he is Principal Scientist and Area Coordinator, Nanomaterial Toxicology Group. He obtained his Ph.D. Biochemistry from University of Lucknow, India in 1991.

Professor Dhawan started the area of nanomaterial toxicology in the country and has recently published a guidance document on the safe use of nanomaterials. His group elucidated the mechanism of toxicity of metal oxide nanoparticles in human and bacterial

cells. His work has been widely cited. He set up a state of the art nanomaterial toxicology facility at CSIR-IITR.

He pioneered the identification of peripheral biomarkers of exposure, effect and susceptibility to xenobiotics. Using DNA damage in lymphocytes as a biomarker of exposure, he has established the reference values for DNA damage in healthy Indian population. He also developed and validated *Drosophila melanogaster* for *in vivo* genotoxicity assessment. These can have far reaching applications in predicting the adverse health effects of drugs and chemicals on human health. He was instrumental in promoting the cause of alternate to animal models in toxicology including *in silico* models.

His work in the area of nanomaterial toxicology has won him international accolades as well and he was awarded two Indo-UK projects under the prestigious UK-IERI programme. He also has two European Union Projects under the FP7 and New INDIGO programmes.

He founded the Indian Nanoscience Society in 2007.

INDIRA GHOSH

Jawaharlal Nehru University



Professor Indira Ghosh has vast experience of working in industry and academia in the field of Biophysics, Computational Biology & cheminformatics leading to aid of drug designing in infectious diseases. She has worked in AstraZeneca for 13 years (1990-2013) in lead designing projects associated with diseases like Tuberculosis and Malaria. Since last ten years her experience has been enriched in academia as Director of Bioinformatics, University of Pune and Professor /Dean, School of Computational & Integrative Sciences, JNU, New Delhi.

She has been actively training human resources in the fields of Bio and cheminformatics and provided 7 Ph.D and 35 M.Sc./M.Tech. project trainees in the field of Computational Biology & Bioinformatics.

She has a Master degree in Physics from Calcutta University and Ph.D. from Indian Institute of Science, Bangalore with a long post doctoral experience in Andy McCammon's lab where she worked as Fulbright scholar during 1983-86. She has been associated with the Royal Institute of Technology and Karolinska Institute, Stockholm, Sweden during 1987-93.

She has been one of the pioneers in propagating education in Computational biology and cheminformatics in Indian Universities and is the member of task force in ICMR (medical informatics) & DeITY (Computational Biology group) which encourage medical professionals and computer science graduates to work in the interdisciplinary research area like Systems Biology & Synthetic Biology.

WORKSHOP LEADERS

P. V. BHARATAM

National Institute of Pharmaceutical Education and Research



Dr. Prasad V. Bharatam is Professor of Medicinal Chemistry at National Institute of Pharmaceutical Education and Research (NIPER), S.A.S. Nagar, India.

Prof. Bharatam, hails from Indian rural environment and highly traditional family background. His strengths are in the oriental training at family and scientific training in schools and colleges.

He obtained masters degree from Visva-Bharati, Santiniketan (1984), and Ph.D. from University of Hyderabad, India (1990).

He spent about four years in American and German universities for research work.

He started his career as a faculty at G.N.D. University, Amritsar and moved to National Institute of Pharmaceutical Education and Research (NIPER), Mohali.

His research expertise is in the design (CADD) and synthesis of computationally designed compounds. He introduced the concepts like 'additivity of molecular fields' and identified new chemical species like 'nitreones'. His work also deals with the computational analysis in drug metabolism, drug toxicity and drug delivery. He guided 20 Ph.D. students and published 180 original research articles.

Various recognitions received by Prof. Bharatam include Alexander von Humboldt (AvH) fellowship (2002), Royal Society of Chemistry (RSC) fellowship (2007), Chemical Research Society of India (CRSI) medal (2008), IBM Faculty award (2007), Ranbaxy Research Award (2008), OPPI Scientist award (2009), Fellowship of AP Academy of Sciences (2012), etc.

MARKUS HEGI

Douglas Connect



Markus Hegi is the Software Development Manager of Douglas Connect, leading and coordinating the software architecture and implementation for the European projects ToxBank, eNanoMapper and EBiSC.

He is also the Founder, CEO & CTO of the Swiss-Indian software company [Colayer] - a social web collaboration platform, which is mainly used in the healthcare industry to coordinate, communicate and for knowledge management.

Markus Hegi architected the cloud SaaS/PaaS platform and leads the implementation. The Colayer core is developed in Switzerland,

where he lives 30% of his time. features and projects are developed in the technology center in Pune (India),

Markus Hegi is active on Social Media and he is also a board member of the [Green Liberal political party] of the Kanton Zürich. He founded and leads the work group Social Media.

Before, Markus worked for Deloitte Consulting Zürich & San Francisco in IT Strategy, Change Management and e-Business.

He obtained an MBA HSG from University St. Gallen (Switzerland), studied Computer Science and Mathematics at FernUniversitaet Hagen (Germany) and Philosophy and Sociology at University of Zürich.

SAMI MUKHOPADHYAY

NovaLead Pharma



Dr. Sami Mukhopadhyay is presently Principal Application Scientist in NovaLead Pharma (erstwhile VLife Sciences Technologies), Pune. He has been associated with VLife Sciences and NovaLead Pharma right from their inception. He specializes in computational chemistry and molecular modelling in Computer Aided Molecular Design (CAMD) both related to drugs and material design. Apart from managing innovation oriented pharma projects related to NCE design, drug repositioning as well as VLife's genotoxicity prediction services for the generic pharma industry, in the materials area, Sami also heads the research projects related to novel

catalyst design for polymerization, several projects in the specialty chemicals, personal, lifestyle and beauty care areas at VLife and NovaLead.

He is also actively involved in developing strategic alliances with industry and academia. He has actively conducted numerous training programs in CAMD for both premiere academic institutes as well as industry through invited lectures, presentations and hands-on training sessions. Sami is actively involved in exploring business opportunities with pharma and non-pharma industry, client requirements capture, client interfacing through technical presentations and interactions and client relationship management.

Dr. Sami has over 18.5 years of industrial experience after Ph.D from IIT Kharagpur in Synthetic Organometallic Chemistry. His earlier experience as senior research scientist includes synthetic chemical product and process development and optimization in Novartis R&D and CAMD work in Tech Mahindra, R&D. Sami has several high impact international research publications to his name.

VARUN KHANNA

Institute of Life Sciences



Dr. Varun Khanna did his post graduation in 2006 with a degree in Bioinformatics from Chaudhary Charan Singh Haryana Agricultural University, Hisar, India. He then received his Ph.D. in Bioinformatics from Macquarie University, Sydney, Australia under the guidance of Professor Shoba Ranganathan. After completing his Ph.D. in 2011, he worked as a postdoctoral fellow in Macquarie University where he was actively involved in the project aimed at analyzing occurrences and co-occurrences of molecular fragments in pharmaceutically important chemical compounds for advancing the knowledge in computational library design

and ligand-based drug discovery. He then moved to University of California, Riverside, USA for another post doctoral assignment. In UC Riverside he was involved in the chemogenomics, data mining project aimed at carrying out a comprehensive selectivity-centric analysis of ligand-target interactions in public activity profile databases such as ChEMBL, BindingDB and PubChem Bioassay.

Currently, he is an Assistant Professor at Institute of Life Sciences, Ahmedabad University, Ahmedabad, India where he teaches Bioinformatics, Pharmaceutical biotechnology and Concepts in computing course to graduate and undergraduate students. His current research interest includes developing novel techniques for computational drug design, chemogenomics, fragment based virtual screening, machine learning and developing android application for biological research. Till date has authored several research papers in international peer reviewed journals and two book chapters.



HOW TO REACH ILS, AHMEDABAD UNIVERSITY

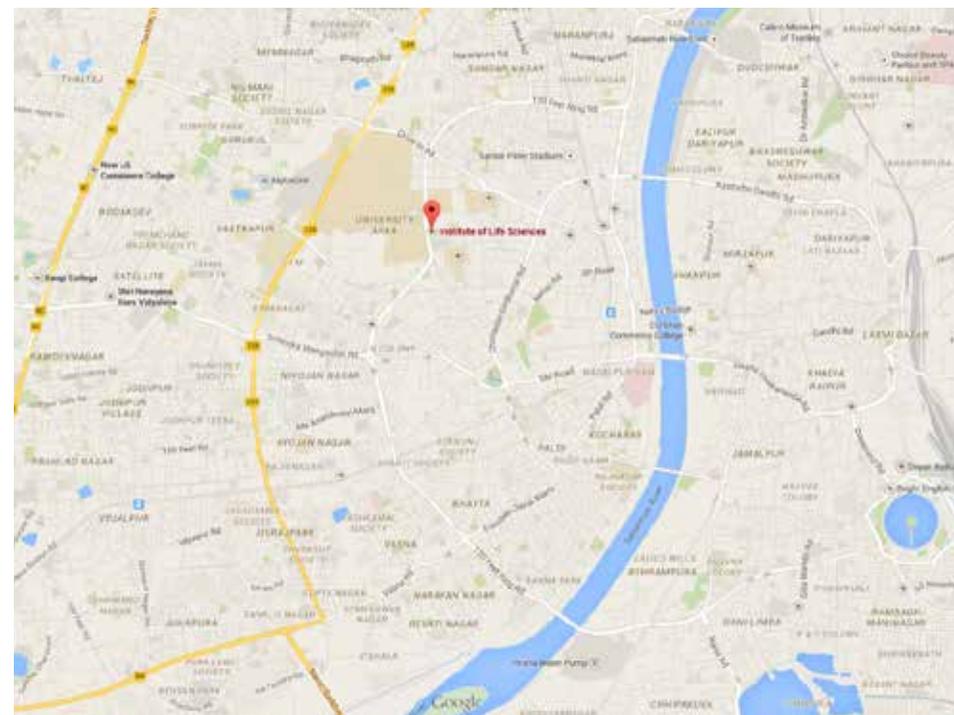
Ahmedabad University is located in Navrangpura.

It is well connected to other parts of the city.

Daily bus services from other parts of the city are provided by state and private bus companies.

Nearest railway station is 'Kalupur' which is at a distance of 5 km from Navrangpura. Airport is around 12 km from Ahmedabad University.

Taxis, autos and bus services to Navrangpura are readily available from the airport and railway station.





INSTITUTE OF LIFE SCIENCES *AHMEDABAD UNIVERSITY*

Institute of Life Sciences (ILS), School of Science and Technology, Ahmedabad University was established in August 2012 with the motto "Nurturing Science, knowledge and Innovation". The institute boasts of three Centres of Excellence (CoE) including VLife Sciences CoE on in-silico technologies. Furthermore, the institute has been set up with well-equipped modern laboratories and classrooms. To encourage research based teaching and project based learning, a world class infrastructure has been established. The institute offers an MSc and a PhD program in Life Sciences. The uniqueness of the MSc program is embedded in its multidisciplinary approach to impart better understanding in rapidly advancing biological sciences. The novel course design has been embedded with topics such as product design and innovation; OMIC technologies (genomics, proteomics and metabolomics); sensors and chips as well as ethical legal and social issues to make students ready for industry as well as academia. Candidates are also selected to pursue 1 year full-time research during 3rd and 4th semester. ILS has strong international, industrial and academic linkages to support students and faculty.

A VARIETY OF SOFTWARE PACKAGES WILL BE AT YOUR DISPOSAL TO WORK THROUGH THE PROBLEMS POSED BY THE INSTRUCTORS.

INTERACTIVE PRAGMATIC WORKSHOPS WITH LEADING EXPERTS AND INDUSTRY PRACTITIONERS...

- ✘ Protein Target & Ligand Modelling
- ✘ Virtual Screening & Docking
- ✘ Pharmacophore Models
- ✘ Consensus Strategies
- ✘ Focused Library Design
- ✘ Molecular Simulation & Binding Energy
- ✘ Predicting ADME & Toxicities
- ✘ Fragment-based Drug Design

YOU WILL HAVE AMPLE OPPORTUNITY TO DISCUSS YOUR PERSPECTIVES AND CRITICISMS OF THE METHODS STUDIED AND YOU'LL TAKE-AWAY KEY NUGGETS OF UNDERSTANDING FROM THESE INTENSIVE SESSIONS.

GROUP WORK & DISCUSSION ON WORKSHOP CASE STUDY PROBLEMS

At the beginning of the week, participants will form themselves into small groups depending on their interests and team diversity. These groups will be given case studies and the associated data and, having agreed on which problem they wish to focus, they will decide on their strategy using the methods and software studied during the workshop. Finally, they will present their results to the rest of the participants for discussion.

JOIN THIS INTERNATIONAL COMMUNITY OF LEADING SCIENTISTS...

Founded in 2003, eCheminfo is an ongoing Community of Practice (CoP) committed to the core value of outreach with diverse groups in the commercial, government and academic sectors for the sharing of best practices and the development of strategies, resources and methodologies that address specific issues in improved drug discovery and productivity.

The network involves a diversity of subject matter expertise comprised of experienced professionals from

the life science and pharmaceutical industry, vendors, research institutes, universities and government.

A strong emphasis on science and innovation in addition to networking and personal contacts and discussion is followed at eCheminfo events. Collaborative research projects furthering drug discovery and safety innovation goals are currently being pursued to advance the creation of a community of research approach to challenging problems and issues.

>> echeminfo.com <<

USE LEADING-EDGE METHODS AND SOFTWARE APPLIED TO DRUG DISCOVERY PROBLEMS. DISCUSS PRACTICAL EXAM- PLES, METHODS AND EMERG- ING TECHNIQUES.

- ✘ Class facilitation, discussions and support led by Community Manager Dr. Barry Hardy and an international faculty team of expert drug discovery application practitioners
- ✘ Use leading drug discovery software packages including OpenEye, PLANTS, Amber, CCG, OpenTox, VLife Sciences
- ✘ Integrating a case study approach and group work throughout the week on methods, datasets, challenging problems and discussion of results obtained
- ✘ One year's membership of eCheminfo included



Community of Practice for
Drug Discovery & Development

REGISTER NOW FOR ECHEMINFO
WORKSHOP WEEK ON

DRUG DISCOVERY DESIGN
METHODS & APPLICATIONS

ORGANISERS

Institute of Life Sciences, Ahmedabad University, Ahmedabad,
India in collaboration with Douglas Connect, Switzerland.

Douglas Connect GmbH
Baermeggenweg 14
4314 Zeiningen
SWITZERLAND

Institute of Life Sciences
Ahmedabad University
University Road, Ahmedabad
INDIA

Douglas Connect
Working communities



WAYS TO REGISTER

✓ Online at

>> events.douglasconnect.com <<

CONTACT PERSON

- ✓ VARUN KHANNA (in India)
- ✓ email: varun.khanna@ahduni.edu.in
- ✓ Cell phone: (+91) 98255 57476

www.echeminfo.com