Latest Advances in Computational Drug Discovery

Session Leaders:
Dr. Paul Hawkins, Dr. Gregory L. Warren and Dr. Christopher Bayly**,**
OpenEye Scientific
Prof. Indira Ghosh, JNU
Sunil Chawla, Seascape Learning

Venue: JNU convention Center -New Delhi
October 29 (Mon) 2012 10am-4pm

JNU in collaboration with Seascape Learning and OpenEye Scientific USA, is pleased to offer an Interactive Seminar on advances in Computational Drug Discovery focused on Shape and Electrostatics.

Key Questions of focus will be:

What are the fundamental molecular descriptors?

How do Shape and Electrostatics improve the science of drug discovery?

How to improve scientific effectiveness in drug discovery process?

Speakers/Moderators:
• Dr. Paul Hawkins**,** Applications Science Group Leader
Dr. Gregory L. Warren, Applications Scientist
• Dr. Christopher Bayly**,** Senior Scientist

An indepth presentation/discussion of advances/issues in the areas of:
• Ligand based design
• Structure based design
• Lead optimization

The Seminar will be followed by software demo/discussion for interested participants who want to get indepth. No computers will be required.

- **References:**

  - http://www.eyesopen.com
  - Schneider, G.; Bohm, H. J. Virtual screening and fast automated docking methods. *Drug Discovery Today* **2002**, *7*, 64−70.
  - Lyne, P. D. Structure-based virtual screening: an overview. *Drug Discovery Today* **2002**, *7*, 1047−1055.
  - Bleicher, K. H.; Bohm, H. J.; Muller, K.; Alanine, A. Hit and lead generation: beyond high-throughput screening. *Nat. Rev. Drug. Discovery* **2003**, *2*, 369−378.
  - Shoichet, B. K. Virtual screening of chemical libraries. *Nature* **2004**, *432*, 862−865.
  - Jorgensen, W. L. The many roles of computation in drug discovery. *Science* **2004**, *303*, 1813−1818.
  - Lengauer, T.; Lemmen, C.; Rarey, M.; Zimmermann, M. Novel technologies for virtual screening. *Drug Discovery Today* **2004**, *9*, 27−34.

Speaker Profiles

About Paul Hawkins, Applications Science Group Leader, OpenEye Scientific

PhD, University of St. Andrews, 1993

Paul got his Ph.D from University in Southampton. After a post-doc in the U.S. and Australia he settled, in New England (Boston) to work in biotech as a medicinal chemist. In this capacity he was involved in a variety of project areas, making a wide range of compounds. After a number of years at the bench he became an applications scientist for Tripos, covering the New England area. Paul has numerous publications and patents to his credit. His professional experience includes OpenEye Scientific, Tripos, Arqule, Paratek & Ariad Pharmaceuticals.

About Christopher Bayly, Senior Scientist OpenEye Scientific

Ph.D. University of New Brunswick, 1991

Starting off with a B.Sc. in Biochemistry, Christopher initially moved into synthetic organic chemistry,. A couple of years later he switched to theoretical chemistry, tying up the synthetic organic work with a Master's degree. He has a doctorate in Theoretical Chemistry . He did his postdoc in Peter Kollman's group at UCSF. Subsequently joining Merck Frosst in Montreal in 1992, he founded and built the Chemistry Modeling and Informatics group there, leading it right through to the very end with the closure of the research site in 2010. He developed new charging method AM1-BCC (with his first PhD student Araz Jakalian) and is best known for his work on molecular polarization with Jean-Francois Truchon.

About Gregory L. Warren, Senior Applications Scientist, OpenEye Scientific

PhD, Massachusetts Institute of Technology, 1994

Greg went to graduate school at MIT where he studied protein crystallography, solution and solid-state NMR in the labs of Greg Petsko and Bob Griffin. He did hid post-doc at Brünger lab at Yale. He worked as a computational chemist at SmithKline Beecham later, to become GlaxoSmithKline.

OpenEye's guiding philosophy is that it is sufficient to accurately quantify the shape and electrostatics of a molecule for the purposes of lead discovery. Following that philosophy, OpenEye provides tools that vastly increase the scale of operation of computational chemistry in drug design. Since there are an almost infinite (10**200) number of feasible drug-like molecules, a productive discovery process will lead to effective drug candidates.

About Seascape Learning. Seascape is an international collaborative engaged in computational science software and related projects in emerging areas of drug discovery, material sciences. Seascape operates from Silicon Valley and India.

About Prof. Indira Ghosh, Professor, School of Computational & Integrative Sciences (earlier called SIT), JNU. Indira is engaged in drug designing since her Ph.D research at I.I.Sc. With a brief Fulbright scholarship post-doc with Prof. J.A.McCammon at Houston she has worked in research institute in an out of country and has 13 years experience at AstraZeneca, Bangalore as leader of the CADD & Bioinformatics. Since 2003 she worked as Director, Bioinformatics center at Pune as a Professor , IBB. In JNU since 2008 she is working as project leader in the COE-DBT supported Center for Computational Biology & Bioinformatics . Her area of research encompasses gene based identification & validation of target, design of compounds for hit to lead phase. Recently her team has been working on an EU-supported FP7 project (OpenTox) on "Toxicity Prediction" which has been completed in 2011.

For Registration Details, please visit http://www.seascapelearning.com/oesymp2012jnu

Registration Process
Please send an email to ighdna@yahoo.com or to Sunil@seascapelearning.com providing us your name, full contact information and background (JRF/SRF/RA working in the research lab or academia or industry) by email or online (www.seascapelearning.com).

NO REGISTRATION FEE , But you are required to register PLEASE.

One may use the following URL for it:
http://www.seascapelearning.com/oesymp2012jnu.html

Maximum person accommodated: 30

Last date for Registration: October 20 2012
An eCertificate will be provided upon successful completion of this Seminar.

Official postal address : Prof. Indira Ghosh, Jawaharlal Nehru University, School of Computational & Integrative Sciences, New Mehrauli Road, New Delhi-110067.

No TA-DA and no accommodation is provided. Please make your own Travel support and accommodation arrangements in/around JNU - New Delhi