

A workshop on Bioinformatics@BioAsia 2012 was organized by NIPER-Hyderabad and Bio Asia 2012 in association with Department of Pharmaceuticals, Ministry of Chemicals and Fertilizers, Govt. of India and Schrödinger on 09th February 2012 at NIPER– Hyderabad campus.



NIPER Hyderabad: National Institute of Pharmaceutical Education and Research (NIPER) is an autonomous body and established under the aegis of Ministry of Chemicals & Fertilizers at Hyderabad as a centre of excellence for higher education, research and development in pharmaceutical sciences. The institute has been declared as an “Institute of National Importance” by Government of India through an Act of Parliament (NIPER ACT 1998 & NIPER Amendment ACT 2007). This institute offers M.S (Pharm) programmes in 4 disciplines viz., Medicinal Chemistry, Pharmaceutical Analysis, Pharmacology & Toxicology and Pharmaceutics. Ph.D. programme in three disciplines viz. Medicinal Chemistry, Pharmacology & Toxicology and Pharmaceutics has been commenced from the academic year 2011-12. From the academic year 2012-13, M. B. A (Pharm) course commences in this institute. NIPER-Hyderabad is mentored by Indian Institute of Chemical Technology, Hyderabad.

Bio Asia 2012: From February 9th to 11th 2012, BioAsia 2012 will unfold its ninth chapter on a vibrant international platform with the theme of “Optimizing Opportunities”. BioAsia 2012 has identified 4 key focus areas – viz., Vaccines, Contract Research, Investments and Intellectual Property Rights (IPR) that will drive synergies amongst key stakeholders and participants. BioAsia 2012 intends to focus on all four key areas in the context of changing trends, continuous challenges, potential for growth and future developments. The forum will witness industry key stakeholders and thought leaders exchange meaningful dialogue, knowledge sharing and provide networking and bio business opportunities besides providing participants an exclusive opportunities to exhibit, launch and showcase their unique strength, products and services.

Schrödinger: Schrödinger is a scientific leader in computational drug design for pharmaceutical and biotechnology research. Schrödinger makes significant investments in R&D, which has led to major advances in the field of computational chemistry. Working closely with its scientific advisory board – a distinguished group of leading academic and industrial scientists who collectively have over one thousand publications with over 50,000 citations – Schrödinger has achieved breakthroughs in quantum chemistry,



molecular modeling, force fields, molecular dynamics, protein structure determination, and docking.



The objective of this workshop is to bring together students, researchers and practitioners interested in the field of Bioinformatics and to demonstrate the recent developments and importance of Bioinformatics and highlight its role in Health Care sector. The prime idea to conduct this workshop is to give training to selected personnel from all over India and highlight the role of Bioinformatics in current scenario. This enables the participants to return to their labs with new ideas, software experiences and best practices to maximize productivity in their own research activities. Workshop groups will study problems with hands-on examples using Bioinformatics software and discuss complex issues highlighted by examples and case studies presented by faculty.

The workshop was inaugurated by the Chief Guest **Dr. Raja Sekhar Vandru**, IAS, Joint Secretary, Dept. of Pharmaceuticals, Ministry of Chemicals & Fertilizers, Govt. of India, **Dr. K. V. Raghavan**, Vice-President, FABA, **Dr. Ahmed Kamal**, Project Director and **Dr. Kolupula Srinivas**, Convener by lightening the lamp. **Dr. Ahmed Kamal** welcomed the gathering and in his



welcome address, highlighted the objective of workshop and demonstrate the recent developments in bioinformatics and highlight its role in current scenario. He briefed about NIPER-Hyderabad and various conferences and seminars conducted at the campus. He also briefed about NIPER new courses which are going to be commenced in the new academic year. The Guest of



Honor, **Dr. K. V. Raghavan** emphasized the crucial role played by bioinformatics in the development of various areas of biosciences. He said that the structure activity design of drugs in bioinformatics plays a major role. Depending upon structure activity design, we can classify the different bioinformatics as biopharmacoinformatics, toxicoinformatics and health informatics. He also said that potential drug targeting has used bioinformatics as an HTS tools for the screening of the new molecule entities and mentioned about the



FABA activities including BioAsia event and upcoming “Conference on Stem Cell Research”. The Chief Guest **Dr. Raja Sekhar Undru** highlighted the importance of such workshops and conferences that help the students to update themselves in the field of the interest. He has given a statistical analysis about amount of expenditure spent on research and said that it was increased from 80 crore to



234 crore over the 15 years in India. But in the foreign R&D sectors the expenditure is from 64 crores to 934 crores, which is many fold investments. He emphasized that the IT and biologics is a new era and that will bring new medicines for the disease for which we have no new medicines. Finally he concluded that “The Future is in Biopharma”. He also launched redesigned NIPER-Hyderabad website. In the inaugural function, Prof. N Satyanarayana, Registrar, NIPERHyderabad; Dr S.S Varaprada Rao, Former BDMA President; Dr P. V Appaji, Executive Director, Pharmexcil; Prof. E Muralidarshan, IIFT; Eminent Speakers, Scientists from IICT and other academic institutes and industry, officials from IDPL, Schrodinger Team, Course Coordinators, Faculty, Staff and Students of NIPER-Hyderabad were present.



Prof. B. Jayaram, Department of Chemistry, IIT, Delhi has delivered a talk on “Genomes to Hit Molecules *In Silico*: A country path today, a highway tomorrow”. He spoke about the importance of databases, aspects of DNA sequence and the way in which drug design software fall short of expectations even if the structures of drug targets are known. He explained the development of all atom energy based methodologies for whole genome analysis (*ChemGenome*), tertiary structure prediction of proteins (*Bhageerath*) and protein/DNA targeted lead molecule design (*Sanjeevini*). He also discussed about how these methodologies can be configured into an assembly line to deliver hit molecules from genomic information.

After the tea break, the session was started with the lecture by **Dr. Anthony Addlagatta**, Senior Scientist, IICT; has delivered a talk on “*Protein crystallography: implications in drug discovery and modern biology*”. The use of protein crystallography in modern biology and drug discovery was discussed. Parameters that will enable non-crystallographers such as bioinformaticians, molecular modelers, protein chemists, medicinal chemists, cell biologists etc. to choose a correct structure for their research were emphasized.



Dr. Ravindranath S Rathore, School of Life Sciences, University of Hyderabad; has delivered a talk on “*Emerging Scenarios in Structure Determinations and Predictions*”. He spoke about homology modeling, threading (fold recognition) and *ab initio* methods as emerging alternative ways of elucidating three-dimensional structures of enzymes and the employment of these predictive methods in rational drug discovery process. He also gave a brief outline of the structure prediction methods, their scope of applications, and a case study.

Dr. Kunchur Guruprasad, CCMB, Hyderabad has enlighten the students by delivering a talk on “*Construction of 3-D model of the Plasmodium falciparum 20S proteasome - exploring the biological and chemical space in the catalytic subunits compared with yeast 20S proteasome inhibitor complexes for rational drug design*” He discussed about The proteasome molecular machinery and its involved in the degradation of misfolded proteins and



short-lived regulatory proteins, besides having a role in cell-cycle control, cell differentiation and metabolic adaptation, and cellular immune response. He also discussed construction of the three-dimensional model of the Pf 20S proteasome and mutations associated with the catalytic subunits likely to confer specificity and that may be exploited for the design of suitable inhibitors.



Dr. G. Madhavi Sastry, Project Manager, Schrodinger Team, & D. E. Shaw India Software Ltd., Hyderabad has delivered a talk on “*Visiting Molecular Docking Algorithms and the Challenges in Predictive Abilities*”. She discussed about conformational search algorithm, scoring function and the chief objectives of a good docking algorithm. She focused on different methodologies and latest trends that have been used to address a few aspects of a docking algorithm. She also discussed different scoring functions based on implicit and explicit solvation methods to account for interaction forces.

The post lunch session was followed by hands on session where the delegates worked on molecular docking, homology modeling and various other tools used in molecular modeling and drug design studies. The participants have expressed their happiness as this is a rare opportunity for them to interact with people from different parts of the country and they are delighted with



the hands on session which helped them to understand the software. During the scientific session and Hands-on training, the delegates were interacted with Speakers about career opportunities in this filed. In the Valedictory Session, Prof. N Satyanarayana, Registrar NIPER-Hyderabad; has chaired the session and thanked the all the organizations including eminent speakers and delegates. He has presented momentoes to Schrodinger team as part of appreciation.

In this workshop, BioAsia 2012 team: Mr. Shakthi Nagappan; Mrs. Paridhi Gupta were involved in the arrangements of this meet. This event was supported by Department of Pharmaceuticals, Govt of India; and Schrödinger team. The Registrar: Prof. N Satyanarayana, Course Coordinators: Dr R. Srinivas, Dr S. Ramakrishna, Dr A. Krishnam Raju; Faculty members: Prof. V. Peesapati, Prof. Nalini Shastry, Dr Bathini Nagendra Babu, Dr. Kolupula Srinivas (Convener), Dr N. Shankaraiah, Dr S. Sunitha, Mr. T. Venu (Co-convener), Dr Narendra Kumar Talluri, Dr S. Gananadam, Dr Satheesh Kumar, Mr. Naveen Kumar, Dr. V. G. M. Naidu, Dr. Md. Arifuddin, Shri M.S.N. Murthy, Shri C. Badrinath and students and supporting staff members of NIPER-Hyderabad have involved actively. The success of this workshop is a collective effort of NIPER-Hyderabad, Indian Institute of Chemical Technology (IICT), BioAsia 2012 and Schrodinger India.



NIPER -Hyderabad

National Institute of Pharmaceutical Education and Research

(Department of Pharmaceuticals, Ministry of Chemicals and Fertilizers, Govt. of India)

Balanagar, Hyderabad, A.P. – 500037, India. Ph: 040-23073741/40

www.niperhyd.ac.in