



National Institute of
Pharmaceutical Education
and Research
NIPER Hyderabad

News Letter on CAD3 – 2010

Summer Workshop on 'Computer Aided Drug Design and Discovery' (CADD/CAD3) -2010 was organized by NIPER-Hyderabad and sponsored by VLife Sciences Technologies Pvt. Ltd., Pune from 30th April to 2nd May 2010.

About 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).



About VLife Sciences: VLife Sciences Technologies Private Limited, Pune is a leading provider of licensed software and research solutions for discovery research projects in a variety of sectors. VLife offers the VLifeMDS® suite for a comprehensive approach to computer aided drug design. The software implements innovative world-class methodologies for three-dimensional molecular structure modeling, simulation, analysis, visualization and prediction.

The objective of this workshop was to demonstrate the recent developments and importance of Molecular Modeling techniques in Drug Design and Discovery. This workshop was targeted towards



Master Students from NIPER-Hyderabad and other Universities, researchers from different institutions and faculty from various pharmacy colleges. The main aim behind this workshop concept was to provide a set of stimulating sessions using advanced molecular modeling techniques that would be useful to students, faculties and researchers working in drug discovery. Besides theory sessions on various topics, hands on experience has also provided to the participants. The workshop was also designed in a manner that would help the participants return to their labs with new ideas, best practices and software experiences that would maximize productivity in their own discovery research activities.



The summer workshop on CAD3-2010 was inaugurated by Dr. Ahmed Kamal, Project Director NIPER-Hyderabad. In his welcome address, he emphasized the importance of molecular modeling techniques in lead identification of drug discovery. He also highlighted the various activities and

recent developments of NIPER-Hyderabad. Dr. Kamal mentioned about the initiation of a Post-Graduate Diploma Course in Pharma Patents Law in association with NALSAR University in short time.

Prof. N. Satyanarayana, Registrar, NIPER-Hyderabad in his welcome address, he enunciated that molecular modeling tools helps to bring down the actual cost and timelines required identifying and optimizing lead candidates. He pronounced the necessity of practical knowledge about the latest techniques to the participants. Dr. K. Srinivas, Convener, CAD3-2010, highlighted the importance of this event. He emphasized



on the specialty of this workshop that had only about 30% theory sessions and the rest was hands-on sessions.



Dr. Sami Mukhopadhyay, Principal Application Scientist, VLife Sciences and Technologies, spoke in the inaugural lecture about the fundamental aspects of Structure and Ligand based drug design molecular modeling approaches in Computer Aided Drug Design. He compared these approaches highlighting their strengths and weaknesses from a practical/real life industrial perspective. He emphasized stepwise experimental validation of computational results for better and more

realistic predictions and suggested future directions in terms of integration of existing CADD approaches with systems biology approach for more holistic and realistic predictions for and interpretations of experimental results. In his 2nd day lecture, Dr. Sami spoke on Virtual Library generation and screening in terms of realistic filters to arrive at better promising lead candidates. He further continued his presentation on different aspects of Chemoinformatics highlighting the importance of Pharmacophore modeling as a key aspect in the search for promising new leads as well as expanding the existing lead application space.

Dr. Gopalakrishnan Bulusu, Principal Scientist, Tata Consultancy Services, Hyderabad, enlightened the participants with his lecture on 'Current trends in Structure Based Drug Design'. He quoted that CADD and system biology should work in synergistic manner. Dr. Ravindra Dayam, GVK Biosciences Pvt.



Ltd. delivered a lecture on "Computer Aided Drug Design: Case Studies. He deliberated on obligation of computational chemistry tools in Drug Design and Discovery. Dr. Ravindra emphasized on the need of safer and novel drugs for

the treatment of HIV / AIDS. He elaborated on the use of computational chemistry tools particularly for structure based pharmacophore models in the identification of inhibitors for human APE1 enzyme.



On 3rd day of this workshop, Dr. Ravi Shekhar, VLife Sciences delivered lecture on Quantitative Structure Activity Relationships. Dr. G. Narahari Shastry, Scientist, Indian Institute of Chemical Technology, Hyderabad delivered an inspiring talk on 'The Impact of Chemistry on CADD Molecular Similarity, diversity and Virtual Screening'. His lecture consisted of various computational approaches employed in rational drug design. He also extended his talk to *de novo* drug design and comparative protein modeling with practical examples. Dr. Shastry stated that any computation requires validation before accepting it.

The responses from the participants were overwhelming. The participants expressed that they benefited a lot not only learning the basic concepts and advancements of Molecular Modeling, but also with hands-on session. One of the participants from NIPER-Hyderabad said that this kind of workshops is essential in learning and getting exposed to latest techniques. An M.Pharm student from one of the pharmacy colleges stated that it's worth attending the workshop. In this work shop, Dr R. Srinivas, Course Coordinator; Dr. N. Shankaraiah, Co-Convener, CAD3-2010; and faculty members of NIPER-Hyderabad, Prof. V. Peesapati, Prof. Nalini Shastry, Dr. B. Nagendra Babu, Dr. A. Krishnam Raju, Dr. Narendra Kumar Talluri, Dr. Md. Arifuddin, Dr. S. Ganadam and Mr. T. Venu were involved actively and made this workshop a successful event to organize this work shop successfully.