NIPER-Hyderabad

News Letter

CAD3 – 2011

Computer Aided Drug Design & Discovery

The Workshop on 'Computer Aided Drug Design and Discovery' (CAD3) -2011 was organized by NIPER-Hyderabad and technical support rendered by VLife Sciences Technologies Pvt. Ltd., Pune from 15th - 17th April 2011. This is 2nd workshop and the 1st workshop (CAD3-2010) of similar kind was conducted during April 30th – May 2nd 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). This institute offers M.S (Pharm) programmes in 4 disciplines vis. Medicinal Chemistry, Pharmaceutical Analysis, Pharmacology & Toxicology and Pharmaceutics. Ph.D programme in this institute commences from July 2011.

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 mainly targeted towards Master Students, Research Scholars, faculty from various Pharma institutes, Universities, Research Institutes and Industries across the country. The main aim behind this workshop 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 would also be provided to the participants.

The workshop was designed in a manner that would help the participants go back to their labs with new ideas, best practices and software experiences that would maximize productivity in their own discovery research activities. Dr. J. S. Yadav, Director, IICT; was the Chief Patron and Dr. Ahmed Kamal, Project Director, NIPER-Hyderabad was Chairman for this workshop. Under the guidance of Prof. N. Satyanarayana, Registrar, Dr Kolupula Srinivas, Convener and Dr B. Nagendra Babu, Co-convener, Faculty and Staff of NIPER-Hyderabad were jointly organized CAD3-2011 workshop.

The workshop on CAD3-2011 commenced with 'Vandemataram' prayer and was inaugurated by Prof. N. Satyanarayana, Registrar, NIPER-Hyderabad. He welcomed the

gathering and in his welcome address, highlighted the importance of CADD techniques in Drug Discovery process. He also stressed the need of advanced molecular modeling techniques to fasten the process of Drug Discovery. He also informed the audience about various activities and recent developments of NIPER-Hyderabad. Dr. Kolupula Srinivas, Convener, CAD3 – 2011, explained about the significance of this workshop and how it would be useful for the participants in their career prospective. Dr. V. Jayathirtha Rao, Scientist, IICT, motivated the students in his brief message by stating that one has to accept and adopt latest techniques and students should stand first to follow. Dr. K. Bhanuprakash, Scientist, IICT, congratulated all the delegates and organizers for having this workshop with eminent speakers and stressed to conduct such workshops for educating younger generations. Dr. R. Srinivas, Course Coordinator, Pharmaceutical Analysis and Scientist, IICT, emphasized the usage of molecular modeling techniques in design and understanding small molecules. He further thanked the Speakers and vLife Sciences Technologies for accepting the invitation and supporting this event. Dr. S. Ramakrishna, Course Coordinator, Pharmacology & Toxicology and Scientist, IICT, stated that these workshops would help to update the knowledge on latest techniques and similar series of workshops would be conducted by NIPER-Hyderabad in future. Dr. Sami Mukhopadyay, Principal Scientist, VLife Sciences Ltd, has addressed the gathering and emphasized the importance of this workshop and their association with the NIPERs. He expressed his interest to support and conduct such workshops in future too.

Dr. J. A. R. P. Sharma, Senior Vice President of GVK Biosciences Pvt. Ltd has given a key note lecture on "Nascent Technologies in Drug Design based on Virtual Methods" He explained in a lucid manner how a modern drug discovery program starts with target selection, followed by hit identification, hit-to-lead transition, lead optimization, and clinical candidate selection. Further, he explained various strategies and challenges faced by Pharma Industry in Drug Discovery and Development.

A thought provocative lecture was delivered by Prof. M. Rami Reddy RR Labs Inc. San Diego, USA. He shared his experience on Use of Computer Aided Drug Design Methods and Structural Bioinformatics in the Discovery of New Class of Clinical Candidates for Diabetes and one FDA Approved Drug for AIDS. He discussed about the use of Structural Biology, Structural Bioinformatics, Chemoinformatics, Computer Aided Drug Design Methods, Medicinal Chemistry and Biology for the discovery of new class of clinical candidates for type-2 diabetes using Fructose 1, 6-bisphosphatase (FBPase) as a target enzyme.

After the tea break, the session was started by *Dr. Anthony Addlagatta*, Scientist, IICT on "A Step before CAD3: Analysis of pdb file". He explained how Protein data bank files form an important component of the computer aided drug discovery process. He mentioned that protein structures which were deposited in the PDB are solved by NMR, X-ray crystallography

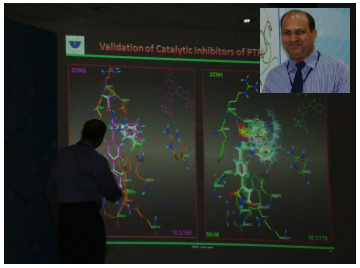
and electron microscopy. He also explained how these structures will be determined and how to judge the quality of a structure before using it for CAD3.

Dr. R. S. Rathore, Scientist, University of Hyderabad delivered a talk on "Structure Prediction Methods in Computer-aided Drug Discovery". He discussed how Computational methods of structure prediction are being routinely employed in structure-based drug discovery to elucidate three-dimensional details of enzymes. He also mentioned that these methods lies in quick and reliable results that are comparable with those obtained from experimental X-ray crystallographic and NMR techniques.

Dr. Sami Mukhopadhyay, Scientist, vLife Sciences Technologies, Pune has delivered an Overview of CAD3. He covered the basic concepts behind structure and ligand based drug design approaches which are key components in CADD techniques. He mentioned about the various Modules of Molecular Design Suit (MDS Software) and their application in some real life industrial case studies.

Post lunch session started by the team members of vLife Sciences. They have demonstrated the use of vLife MDS Software in molecular modeling, Homology and Protein Structure Analysis using a typical case study as human COX-2 target and NSAIDs set of ligands. All the major aspects of BLAST, homology modeling and model validation methods were covered in detail. After the demonstration, Hands-on experiments session was conducted in the Molecular Modeling Lab.

The second day of the work shop was started with an enlightening lecture by Dr. Guru Prasad on Modeling Protein Three Dimensional Structure from Sequence . He explained how bioinformatics plays a vital role to find drug target, about Venn diagram used to describe the properties of amino acid residues with few case studies. Dr. Sreedhara R. Voleti of ILS, Hyderabad has given a talk on "Structure Based Application in Drug – Discovery". He explained how the Structural aspects (ligand or protein) will largely help perform rational drug discovery, and a culmination of ligand interactions with the large biological systems can lead to informed designs of small molecules with synthetic feasibility, intellectual property, and more importantly, cost cutting. Dr. Sami Mukhopadhyay has delivered an educative talk on Virtual Library Generation and Screening. The importance of Virtual screening tools to short list the most promising lead candidates was brought out through different realistic virtual screens were covered by him.



Dr. Raveendra Dayam, Associate Director – Informatics, GVK Biosciences Private Limited has given an extensive talk on "Structure Based Drug Design: Fragment Based Approaches". He discussed the fragment properties, metabolic stability, pharmacokinetic filter to illuminate and how to generate fragment libraries and also how to connect fragments. The post lunch session was dealt with Demonstration and Hand-on experience on Molecular Docking, Virtual screening, Pharmacophore mapping etc. The broad scope of Chemoinfomratics with emphasis on the two key aspects of realistic query generation and appropriate data base search was covered in this session. Techniques of Pharmacophore Modeling were dealt with its growing importance to real life projects in CADD. Further key concepts of Molecular Docking together with strengths and weaknesses of scoring functions were discussed.

The third day of CAD3-2011 was commenced with an introductory lecture on Quantitative Structure Activity Relationships (QSAR) by Dr. Kundan Inagle, vLife Sciences. The key aspects of 2D, 3D QSAR and vLife GQSAR were taken by him. Dr. Devesh Kumar, DST-Ramanujan Fellow, IICT has delivered a lecture on Drug Metabolism by CYP450: A tale of multistate reactivity. He has discussed about the history and biodiversity, biological activity of CYP450. Different models that explained the functioning of en enzyme catalytic cycle of P450 and kinetic isotope effects were discussed in a lucid way. Demonstration on QSAR methods and few case studies related to it were covered by him. The post lunch session was exclusively dedicated for Hands-on training on CADD techniques and especially 2D and 3D QSAR methods.

The responses from the participants were overwhelming. During the theory and training sessions, the delegates were very attentive. Mr. Amit, vLife Sciences, stated that CAD3-2011 workshop is organized in an elegant manner and the delegates are also very serious to learn CADD techniques. The participants expressed that it is a rare opportunity for them and the training given in this workshop is very informative, practical and effective. The delegates stated that they benefited a lot not only learning the basic concepts and advancements of Molecular Modeling, but also with hands-on experiments session. One of the participants from IICT said that this kind of workshops is essential in learning and getting exposed to latest techniques. One Master student conveyed that it's worth attending the workshop and in fact the training received at CAD3-2011 is fulfilled his course curriculum. In this work shop, faculty members of NIPER-Hyderabad, Dr. Bathini Nagendra Babu, Dr. A. Krishnam Raju, Dr. Sunitha, Dr. Narendra Kumar Talluri, Dr. Shankaraiah, Dr. S. Gananadam, Mr. T. Venu, Dr. Satish Kumar, Mr. Naveen Kumar, Mr. Sunil Tripathi, Dr. Md. Arifuddin and senior faculty members Prof. V. Peesapati, Prof. Nalini Shastry and Shri M.S.N. Murthy and other staff members were involved actively and made this workshop a successful event of NIPER-Hyderabad

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