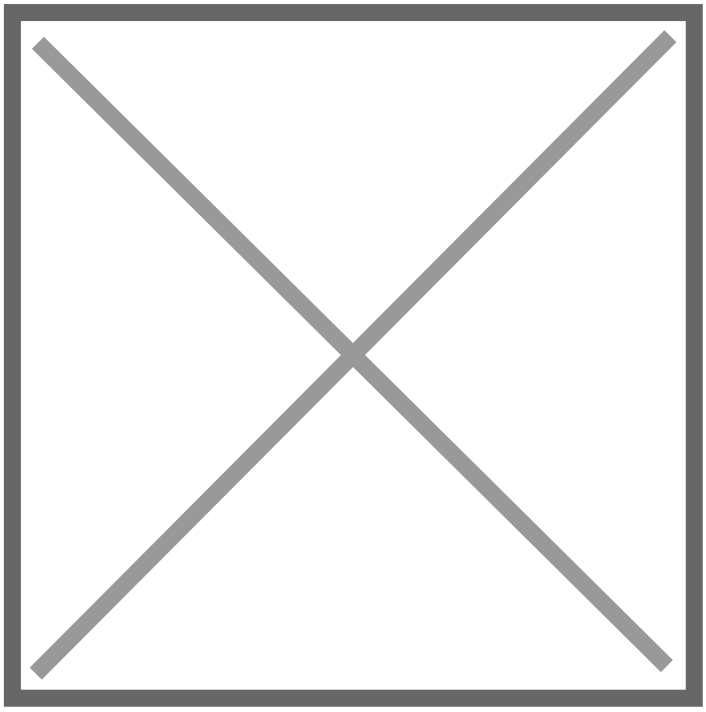
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Virtual connect for real life drugs

07 March 2012 | News



Computeraideddrug Software packages ranging from modeling programs to virtual reality are helping scientists explore structural options and make predictions about the properties of new compounds

Genesis

In early 1980s, computer-aided drug discovery was found to be too ahead of its time. But the scenario has changed since then as there is a tremendous transformation in the field of drug discovery in the last 20 years. In the post genomic era, rational drug discovery is a major approach for discovering and designing new drugs.

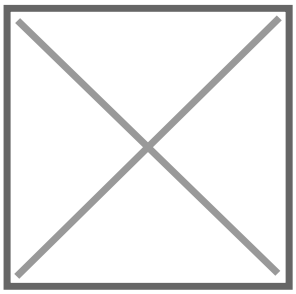
The Technology

The exciting thing about computational tools is their ability to provide atomic level insights into observed molecular interaction and relation to biological data. Dynamic simulations give valuable insights into mobility of molecular interactions for design. These tools are used for molecular design of hits, leads and optimization of leads with better profile as drugs. The molecular docking, dynamics, pharmacophore modeling and virtual screening approaches are important in drug design.

The Impact

Integration of data and analytical technology development around molecular, biological, clinical and other scientific data will be an opportunity for both drug design and translational medicine. The promising areas are systems biology for new target identification, biomarker identification and clinical data analysis leading to personalized medicine. The goal remains generating a reliable computer suggestion of a drug molecule based on the genome card and symptoms of the patient in the least possible time.

Computational tools can save up to 20 percent on the cost and time involved in drug discovery, which otherwise is prohibitively expensive. Since the drug target identification involves finding biomolecules that are responsible for the suppression of pathways, computers can help to generate cause-to-effect simulations with inputs from 'omics' (genomics, transcriptomics, proteomics and metabolomics).



Dealing with data

Huge data generated by the biopharma companies from failed drugs and molecules that have failed in different phases of clinical trials are very important to develop in silico models for drug discovery. In the Indian context, drug discovery in academic labs in collaboration with industry has resulted in new technology development. Packages such as EduSAR from V-life Sciences and Biosuite from TCS are promising examples. Computational platform AVADIS from Strand Life Sciences for target and biomarker identification is well-known. Also, Dr Raghava's group at IMTECH, Chandigarh, has developed a software package, VaxiPred, in collaboration with New Delhi-based Biomantra. Bangalore-based Geschickten Biosciences has collated all its sophisticated algorithms and tools into a cloud-based platform for managing, analyzing and visualizing next generation and third generation genomics data. The company, in 2011, launched two cloud solution tools called 'iOmics' and 'Release: beta version'.

The Gene to Drug software suite developed at the Supercomputing Facility for Bioinformatics, at the Indian Institute of Technology, New Delhi, accessible over the Internet free, comprises genome analysis programs (Chemgenome), protein structure prediction programs (Bhageerath) and computational tools for drug design (Sanjeevini). Two spin-off companies from IIT, LeadInvent and Novo Informatics, have utilized few of these technologies to design novel biological softwares that may help to solve various health issues.

The success of open source models in information technology (web technology and the linux operating system) and biotechnology (human genome sequencing) gave birth to Open Source Drug Discovery (OSDD)Â from the Council of Scientific and Industrial Research. The consortium is spearheading the response to solve problems associated with discovering novel therapies for neglected tropical diseases

Rahul Koul in New Delhi