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National Level Conference on Recent Approaches in Drug Design

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The focal theme of National Level conference Recent Approaches in Drug Design with following objectives.

- To identify global challenges in Drug Design
- To develop an interaction with scientists in the field of Drug Design
- To develop innovative and creative tools in Drug Design
- Harmonization of Pharmaceutical education and research in Drug Design

Typically a drug target is a key molecule involved in a particular metabolic or signaling pathway that is specific to a disease condition or pathology or to the infectivity or the survival of a microbial pathogen. Some approaches attempt to inhibit the functioning of the pathway in the diseased state by causing the target molecule to stop functioning. Most commonly, drugs are organic small molecules produced through chemical synthesis, but biopolymer-based drugs (also known as biologics) produced through biological processes are becoming increasingly more common. In addition, mRNA-based gene silencing technologies may have therapeutic applications. There are two major types of drug design. The first is referred to as ligand-based drug design and the second, structure-based drug design. Alternatively, a quantitative structure-activity relationship (QSAR), in which a correlation between calculated properties of molecules and their experimentally determined biological activity, may be derived. These QSAR relationships in turn may be used to predict the activity of new analogs. Structure-based drug design (or direct drug design) relies on knowledge of the three dimensional structure of the biological target obtained through methods such as x-ray crystallography or NMR spectroscopy. The 3D structures of biomolecular targets are obtained from X-ray crystallography and NMR. The basic inputs for this step are the 3D structure of the protein and a pre-docked ligand in PDB format, as well as their atomic properties.

Computer-aided drug design uses computational chemistry to discover, enhance, or study drugs and related biologically active molecules. The most fundamental goal is to predict whether a given molecule will bind to a target and if so how strongly. Molecular mechanics or molecular dynamics are most often used to predict the conformation of the small molecule and to model conformational changes in the biological target that may occur when the small molecule binds to it. Molecular mechanics methods may also be used to provide semi-quantitative prediction of the binding affinity. Another important case study in rational drug design is imatinib, a tyrosine kinase inhibitor designed specifically for the bcr-abl fusion protein that is characteristic for Philadelphia chromosome-positive leukemias (chronic myelogenous leukemia and occasionally acute lymphocytic leukemia). Imatinib is substantially different from previous drugs for cancer, as most agents of chemotherapy simply target rapidly dividing cells, not differentiating between cancer cells and other tissues.

Since the late 1980s there have been striking advances, fueled by large increases in both industrial and NIH-funded academic research, that have revolutionized drug discovery. This period has seen the introduction of high-throughput screening (HTS), combinatorial chemistry, PC farms, Linux, SciFinder, structure-based design, virtual screening by docking, free-energy methods, absorption/distribution/metabolism/excretion (ADME) software, bioinformatics, routine biomolecular structure determination, structures for ion channels, G-protein-coupled receptors (GPCRs) and ribosomes, structure/activity relationships (SAR) obtained from nuclear magnetic resonance (SAR by NMR), fragment-based design, gene knockouts, proteomics, small interfering RNA (siRNA), and human genome sequences. The result is a much-accelerated progression from identification of biomolecular target to lead compound to clinical candidate.

On behalf of S.M.B.T. College Of Pharmacy, Dhamangaon, Nasik and Savitribai Phule Pune University and Local organizing committee , we extend a heartly welcome to all the guests and delegates to Dhamangaon to participate in the National Level conference Recent Approaches in Drug Design and make it a great success.

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