Partha Palit, Med chem 2013, 3:4
http://dx.doi.org/10.4172/2161-0444.S1.009

OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference on
Medicinal Chemistry & Computer Aided Drug Designing
October 15-17, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

Molecular computer modeling and docking is a new technological tool and as well as gift for drug discovery: Bridging research laboratories and clinics

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Several life threatening diseases such as cancer, diabetes, Alzheimer's, asthma, arthritis and infectious diseases involve malfunctioning of enzymatic or receptor based proteins. Drugs (small molecules) are required to rectify such metabolic disorders through ligand-protein binding by modulating effects. Screening and experimental works of such chemical compounds as drugs, needs time, money, scientific barriers and challenges. Recently, identification of potential molecular targets for drug discovery and development has achieved through exploitation of emerging structural biology, "rational" drug design, screening of chemical libraries. Hit compounds are explored through computer molecular modeling and docking with their exact target enzymes and receptors without evaluation of blind *in vitro* high-throughput random screening. Accurate prediction of exact lead optimization includes determination of scoring functions (descriptors), free energy calculation, investigations of active binding mode and pocket using GOLD, GLIDE AUTODOCK-4. Hence molecular docking based lead identification may reduce the limitations associated with tedious experimental high-throughput large scale screening and guide to elucidate the mechanism of action of new drug molecules. Additionally *in silico* ADMET screening, "druglikeness", have also been resolved various scientific hazards related to drug discovery process and smoothen the avenues to reach the destination of getting blockbuster drug molecule. Here we present the pivotal role and benefits of computer assisted rational drug design through demonstrations of results of docking, ADMET and "druglikeness" of synthetic compounds, generic drug molecules(new uses of old drugs) and isolated phyto molecule and their co-relation with experimental datas. Integration of two major categories: the structure of the protein and the biological and physicochemical properties of bound ligands enhance the reliability and efficiency of these exciting techniques.

Biography

Patha Palit has completed his Ph.D. in 2010 from Indian Institute of Chemical Biology in Pharmacy and working as Assistant Professor in Dr. B.C.Roy college of Pharmacy and Allied Health Sciences for near about 5 years. He is an awardee of Fast Track Young Scientist from Department of science and technology, Govt. of India. He was awarded with gold medal for securing first class in University from Jadavpur University. He has published 9 international papers in reputed journals and has one patent.

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