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Short Communication

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In Silico Technologies in Drug Design

Gowthami Bainaboina*

Abstract

In Silico technologies are developed particularly as an alternate to animal experimentation. In Silico drug design is performed in computers using computational software is known as in silico drug design. In Silico is an expression used to perform on computer stimulations. Since electronic chips used in the computers are usually made up of silicon. It is to analyze the target structures for possible binding sites. And it is used for candidate molecules, checking for their drug likeness.

Drug Design: It is the inventive process of finding new medication based on the knowledge of a biological target and the selected knowledge design should be organic small molecule , opposite charge to the biological target. In the drug design the molecule will interact with target that bind to the target , and it activates or inhibits the function of bio molecule such as protein.

Keywords

Insilico; Drug design; Ligand; DNA sequence

Types of Insilico drug design includes

Ligand based drug design: Ligand is simply a molecule that binds to another. Often a soluble molecule such as neurotransmitters or hormone that bind to a receptor. In this type the receptor is unknown and but the ligand is known. Ligand based drug design relies on the knowledge of the other molecule that bind to the biological target .It defines the minimum necessary structural characteristics molecule must possess in order to bind the target. In Ligand based screening a candidate ligand can be compared to the pharmpacophore model to that determine whether it is compatible with it and therefore likely to bind.

Structural based drug design: It use the structure of biological targets, the drugs that are bind to the target by various designs. It relies on the knowledge of 3-D structure of the biological target obtained through various methods such as NMR spectroscopy, X-ray crystallography ,Homology modeling.

Computer Aided Drug design: Is used to predict the receptor binding site for a protein drug molecule , and used to identify probable binding site and that avoid testing of unwanted chemical which are having no biological activity.

Computer aided learning deals with the range of software which stimulates the animal experiments. The most commonly used software in India are Ex-Pharm, X-cology. Computer models are most frequently used for screening, such models cannot replicate complicated interaction in whole system. Final testing depends on studies in animals, sometimes it is required by law. By using in-silico approaches it is possible to reduce the total number of experimental animals in drug discovery and development.

Insilico Toxicology

Insilico toxicology is an area of active development and great potential. A prediction of potential toxicology requires several stages such as Collation and organization of data available for the compound, information for related compounds. An assessment of the quality of the data. Generation of additional information about the compound using computational techniques at various levels of complexity. Use of an appropriate strategy to predict toxicology that is a statistically valid method which make the best use of all available information.

Some software's used in the drug design are

Sanjeevini: A complete drug design software.
DNA Sequence to structure
Drug DNA Interaction Energy server
Molecular Volume calculator.
Binding Affinity prediction of protein- Ligand server.

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Author Affiliation Top

Department of Pharmacy, QIS College of Pharmacy, AP, India

***Corresponding authors:** Gowthami Bainaboina, Department of Pharmacy, QIS College of Pharmacy, AP, India Mobile:+918500024898; E-mail: gowthamibainaboina@gmail.com

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