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Drug Designing: Open Acccess

Perspective

Drug Discovery Methodologies and its Design

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DESCRIPTION

The process of generating new drugs requires a significant investment of time and money, which makes it a significant challenge for the pharmaceutical sector. Computer-aided drug design is a widely utilised technique to reduce the cost and time for the Computer-Aided Drug Design (CADD). CADD makes it possible to focus studies more effectively, which helps speed up and lower the cost of developing new medications. Structure-Based Virtual Screening (SBVS), one of the most promising *in silico* methods for drug design, is reliable and practical in this context.

SBVS employs scoring functions to determine the strength of the non-covalent interactions between a ligand and a molecular target in an effort to forecast the optimum way for two molecules to engage and create a stable complex. Therefore, the primary factor determining SBVS software's success or failure is its scoring functions. It is possible to get different results from different software using the same input since there are numerous software applications that are used to perform SBVS, and because they all employ different algorithms. Consensus Virtual Screening (CVS), a novel SBVS technique, has been applied in certain research during the past ten years to improve SBVS accuracy and lower the number of false positive results obtained.

The availability of a 3D structure of the target protein is a need for using SBVS. The 3D structures of molecules are kept in a few virtual databases, like the Protein Data Bank. The 3D structure cannot always be obtained experimentally, though. In this case, a protein's three-dimensional structure may be predicted from its amino acid sequence according to the homology modelling methodology. An overview of the difficulties in performing SBVS using CADD tools, the areas where CADD tools help SBVS, a comparison of the most popular tools, and the current approaches taken to shorten the time and expense of the drug development process. The Drug Discovery Methodologies are synthesis, characterisation, validation, optimization, screening, and tests for therapeutic efficacy are all parts of this process.

Screening strategies used in drug discovery

Drug development using high-throughput screening; Early-stage drug discovery frequently uses High-Throughput Screening (HTS). HTS is used to identify "hit" molecules from huge compound libraries, which might contain thousands of molecules, that have action against an interest target. When a hit molecule is discovered, it is verified and developed to create a lead compound with increased selectivity and potency, which can then be investigated further to find a possible drug candidate for preclinical testing. Robotics, liquid/microplate handling systems, and microplate readers are used in HTS to find, monitor, and quantify the events. Additionally, it needs specific software for data processing and instrument control.

High-content screening is the next step in processing after high-throughput screening; According to Janos Kriston-Vizi, group leader of the Bioinformatics Image Core (BIONIC) at the Laboratory for Molecular Cell Biology. In the 1990s, automated fluorescence microscopy and multititre plate high-throughput assays came together to highlight the complex subcellular morphological and intensity-based readouts that enable examining variations in a cell population as opposed to a single population-averaged readout per perturbation.

Fragments Based Drug Discovery (FBDD)

Fragment-Based Drug Discovery (FBDD), also known as the bottom-up technique, is another well-known method for finding new drugs. FBDD uses smaller libraries with hundreds of low-complexity compounds or "fragments," as opposed to HTS campaigns that screen vast libraries of complex compounds. FBDD requires less money for research than HTS. Computer-Aided Drug Design (CADD) is a widely utilised technique to reduce the cost and time for the medication development process. Structure-Based Virtual Screening (SBVS) is one of the most promising in silico methods for drug design. CADD makes it possible to focus studies more effectively, which helps speed up and lower the cost of developing new medications.

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