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Carbon Nanotubes Contribution to Medical Technology

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Introduction

For the discovery of hits, the generation of leads, and the expedited development of high calibre drug candidates, a wide range of medicinal chemistry methods can be applied. Structure-based drug design (SBDD) techniques are getting more potent, adaptable, and popular. This review summarises recent advancements in structure-based virtual screening and receptor-based pharmacophores, highlighting successes as well as difficulties, as well as the importance of structure-based lead optimization, with a focus on recent instances of fruitful applications for the discovery of novel active substances. Proteins and small-molecule modulators form intricate and numerous noncovalent intermolecular interactions that are essential for the functioning of biochemical reactions and cellular systems. The design of small molecules that are capable of regulating or modulating specific target functions in the body that are closely linked to human diseases and disorders is made possible by an understanding of the structural and chemical binding properties of significant drug targets in biologically relevant pathways. This is done through multiple intermolecular interactions within a well-defined binding pocket. The identification of promising hits for additional optimization is generally a significant issue for academic and pharmaceutical laboratories. Despite the inherent nature of trial-and-error in drug discovery, logical ideas and contemporary computer tools are now frequently used for lead selection and optimization [1].

Description

Structure-Based Drug Design (SBDD), also known as the use of three-dimensional (3D) protein structure information in the synthesis of new biologically active compounds, is an approach that university and pharmaceutical research facilities utilise all over the world. For structure-based investigations to be creative and knowledge-driven, a thorough understanding of the spatial and energetic factors that influence the binding affinities of protein-ligand complexes is a crucial prerequisite. Renin is an aspartyl protease that regulates blood pressure, and it has been thought that inhibiting it is a viable way to provide new, alternative treatments for hypertension. A crucial element of medicinal chemistry, the knowledge produced can be used to iteratively design new ligands with enhanced features and characteristics. In order to successfully optimise leads, 3D quantitative structureactivity relationships (3D QSAR) methodologies are one of the most crucial techniques that can be used. In this context, 3D QSAR models are developed to provide a reasonable basis for the creation of novel promising compounds by explaining the links between the intermolecular interactions associated to the 3D conformations of a group of structurally related molecules and their experimental activity [2,3].

In the early phases of any drug development endeavour, it is essential to identify promising hits and produce high calibre leads. The hunt for new drug candidates with a mix of improved pharmacodynamic and pharmacokinetic qualities has a strong foundation thanks to recent developments in medicinal chemistry at the intersection of chemistry and biology. Despite the effects of recent technological and scientific advancements, the cost and time required for drug discovery have increased during the same period of time. Small organic molecules that act on certain therapeutic targets are in high demand because to the extensive use of combinatorial chemistry and HTS for the development of lead compounds. These technologies concentrate on the production of a massive quantity of molecules along with the biological screening of a massive quantity of samples. However, there is a clear paradigm change from the random screening of collections of compounds to a more rational procedure, which would directly affect the success rate of NCE generation due to the constant demand to cut drug development time and costs. The pharmaceutical business faces a number of difficult issues, one of which is finding novel NCEs from a vast pool of real and hypothetically potential chemicals. The use of computational tools can rationally enhance several stages of the drug discovery process [4,5].

No matter where the small-molecule database came from, screening libraries typically include a lot of molecules with a wide range of chemical compositions. Several molecular filters might be employed in the significant library design procedure to cut down on the quantity of compounds that must be screened. In order to direct the selection of compounds with lead-like, fragment-like, and drug-like qualities, common filtering techniques are versions of Lipinski's rule of five that incorporate physicochemical and pharmacokinetic data. The chemical space can also be condensed by identifying the precise qualities necessary for ligand binding or by considering the molecular characteristics displayed by a series of modulators with proven biological action. The main objective of SBVS is to locate molecules that are compatible with the target receptor in terms of shape, hydrogen bonding, electrostatic interactions, and hydrophobic interactions. There is a need for accurate methods for predicting the orientation and conformation of the ligand within the binding cavity of the macromolecular target. The quality of the fit or the computed binding affinity, which are linked to each projected binding mode, must next be thoroughly evaluated. However, creating completely adequate docking algorithms and scoring mechanisms for VS methods still presents numerous difficulties. The main challenges are exploiting ligand shape and protein flexibility, handling desolvation, integrating water molecules, and computing ligand-receptor binding energies [1,2].

Conclusion

Numerous new targets and prospects for drug discovery have been made possible by the explosion of genomic, proteomic, and structural knowledge. The process of finding new drugs nowadays is getting more and more information-driven. New technologies and approaches for NCE design have proliferated greatly in recent years. Modern knowledge-based approaches that use structural data from both targets and ligands include virtual screening and pharmacophore modelling. They are helpful resources for discovering novel molecules with comparable biological activity or for enhancing the potency, affinity, or selectivity of desired active substances. Due to the accessibility of databases containing millions of commercially available compounds and the 3D structures of several target molecules, the application of these drug design methodologies has significantly increased in recent years.

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Conflict of Interest

The author reported no potential conflict of interest.

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