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Drug Designing: Open Acccess

Opinion Article

# Three Dimensional Structure-Based Rational Drug Design

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## DESCRIPTION

Drug design, also known as rational design, and it is the inventive method for developing new medications using information about a biological target. The design of small molecules that are similar in charge and shape to the biomolecular target with which they interact and will bind is the basis of drug design. Computer-aided drug design is the name given to this kind of modeling. Structure-based drug design is a type of drug design that uses information about the target biomolecule's three-dimensional structure. Numerous diseases, including cancer, constantly pose a threat to human life. As a result, the best drugs are always in high demand. An effective method of drug development is necessary to meet the requirements of ideal drugs. Drug development is a difficult, time-consuming, and costly process that requires careful consideration of numerous factors. Drug development necessitates a number of multidisciplinary approaches to meet these obstacles, these methods, taken together, would be the foundation of rational drug design. A biomolecule that plays a role in disease-specific metabolic or signaling pathways is a drug target. A biomolecule, such as the epidermal growth factor receptor, that is frequently altered or deregulated in cancer is a prime example of a drug target. By communicating through protein-protein or protein-nucleic acid interactions that result in the propagation of signaling events or the modification of metabolic processes, biomolecules play a crucial role in disease progression. Therefore, modulating these biomolecules' biological functions would be beneficial and could be accomplished either (i) by inhibiting their function with small molecules whose competitive binding affinity is greater than that of their natural ligands that bind to the active sites (within the biomolecules) or (ii) by inhibiting the relatively less studied bimolecular interactions by small molecules between the biomolecules (iii) by activating biomolecules (for the combined normal functions) that are functionally deregulated in some diseases, such as cancer, or (iv) to stop cross talks between biomolecules. Even for established targets, it is challenging to develop a lead molecule and an effective drug (small molecules with desired properties).The availability of biomolecule 3D X-ray or NMR structures, docking tools, and computer-aided methods have all contributed to a recent surge in drug discovery. The Protein Data Bank (PDB) currently contains approximately 57,558 3D structures, but even this large number is negligible. There are multiple structures bound to various molecules in some biomolecules. Many important targets' 3D structures are still unknown. The number of molecules that resemble lead drugs is also relatively low. As a result, in order to solve the issues that are associated with the drugs that are on the market today and have been developed solely using the strategy of structure-guided drug design, an improved method of rational drug design is required. There are two broad categories of rational drug design: A) Creation of biomolecules (proteins or nucleic acids) with known functional roles in cellular processes and 3D structural information, small molecules with desired properties for targets. The pharmaceutical industries make extensive use of this well-established drug design strategy. B) The creation of small molecules with predetermined properties that are targeted at targets' cellular functions and structural aspects. When new lead drugs are discovered, rational design is used. The significant advancements in computer science, statistics, molecular biology, biophysics, biochemistry, medicinal chemistry, pharmacokinetics, and pharmacodynamics over the past few decades are primarily to blame for its rapid growth. The fact that rational drug design utilizes all known theoretical and experimental knowledge of the system under study to develop potential drug discovery leads is a promising feature. In the end, the goal of using information about the system's molecular foundation is to save time, money, and labor during drug discovery.

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