Abstract

Structure-based drug design (SBDD) is a crucial method in modern drug discovery that uses the 3D structures of biomolecules to develop novel drugs. By focusing on the molecular architecture of target proteins, SBDD

such as molecular docking and dynamics, applications in various therapeutic areas, and challenges faced in its implementation. The article highlights the transformative role of SBDD in personalized medicine, with a focus on

Ke d : Structure-based drug design; Drug discovery; Molecular docking; Protein-ligand interactions; Drug design; Computational chemistry; Targeted therapy; Personalized medicine

I d c

Drug discovery has evolved over decades, shi ing from empirical trial-and-error methods to more rational, data-driven approaches. One such approach, structure-based drug design (SBDD), represents a groundbreaking strategy that utilizes detailed 3D structural information of biological macromolecules [1] to design drugs that can interact precisely with their targets. is technique is based on the principle that the function of proteins (the primary targets of drugs) is intimately related to their three-dimensional shape. By understanding the molecular structure of these targets, researchers can design small molecules that bind e ectively to the protein's active site, altering its function and o ering therapeutic bene ts.

e advent of high-resolution techniques like X-ray crystallography, Nuclear Magnetic Resonance (NMR) spectroscopy, and Cryo-Electron Microscopy (cryo-EM) has made it possible to obtain detailed structural information about proteins [2]. Coupled with computational tools such as molecular docking and molecular dynamics (MD) simulations, SBDD enables the identi cation of potential drug candidates more e ciently, minimizing the time and resources spent in drug development. is approach is particularly bene cial in the design of targeted therapies, where drugs are developed to speci cally target disease-related proteins, leading to higher e cacy and reduced side e ects.

is article outlines the core principles of SBDD, key methodologies, and its diverse applications, focusing on how this approach has revolutionized the development of modern therapeutics.

P c e f c e-ba ed d de :

SBDD operates under the assumption that understanding the structural characteristics of a target protein—particularly its active sites—is essential for designing drugs that can bind e ectively [3]. e drug, or ligand, must t into the target's binding site in such a way that it in uences the protein's biological function, either by inhibiting or activating it.

e process of SBDD generally follows these steps:

Ta e de ca : e rst step is to identify a disease-related

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used in virtual screening, which speeds up the process of identifying promising drug candidates.

M ec a d a c a : Molecular dynamics (MD) simulations are used to study the behavior of molecules over time. By simulating the motion of atoms and molecules, MD simulations help researchers understand how a ligand and its target interact dynamically, providing insights into the stability and exibility of the protein-ligand complex. is approach enhances the accuracy of drug design by modeling real-world conditions.

S c e-ac e a (SAR): SAR analysis involves studying the relationship between a drug's chemical structure and its biological activity. rough iterative modi cations of lead compounds, SAR analysis helps to identify key structural features [7] that contribute to the drug's binding a nity and selectivity, optimizing its therapeutic potential.

H - c ee (HTS): HTS is o en employed in conjunction with SBDD to screen large chemical libraries for compounds that show promise in binding to the target protein. Although HTS is traditionally associated with ligand-based drug design, combining it with SBDD techniques ensures a more targeted and informed selection of compounds for further optimization.

A ca f S c e-Ba ed D De

Ca ce e a : SBDD has proven invaluable in the development of targeted cancer therapies. For instance, the design of tyrosine kinase inhibitors (TKIs) that target speci c mutations in cancer cells has led