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Commentary

Fragment-Based Drug Design: A Promising Approach to Accelerate Drug Discovery

Mohan Krishna*

Department of Pharmaceutical Technology, Jadavpur University, Kolkata, West Bengal, India

DESCRIPTION

Fragment-Based Drug Design (FBDD) is an innovative approach to drug discovery that involves the identification and optimization of small molecular fragments that can interact with a biological target of interest. These fragments serve as building blocks that can be combined and modified to produce potent and selective drug molecules.

The traditional approach to drug discovery involves screening large libraries of compounds against a target of interest, but this approach can be time-consuming and costly. FBDD, also starts with smaller compounds and builds up, potentially leading to a more efficient process.

FBDD typically begins with the identification of small molecule fragments that bind to the target of interest using techniques such as X-ray crystallography, NMR spectroscopy, or computational methods. Once these fragments have been identified, they can be optimized through constant cycles of design, synthesis, and testing. By repetitive modifying and linking together these fragments produces larger and more complex compounds that retain the binding affinity and selectivity.

One advantage of FBDD is that it can help overcome challenges associated with traditional drug discovery methods. For example, it can help overcome challenges associated with identifying small pockets on the surface of proteins that may be difficult to target with larger molecules. Additionally, FBDD can help to identify the issues with off-target effects and toxicity that can arise with larger and less selective molecules.

There are several successful examples of FBDD in drug discovery, including the development of vemurafenib, a drug used to treat melanoma. Vemurafenib was developed through FBDD, which identified a small molecule fragment that bound to the target protein, B-Raf. By using this fragment as a starting point for building larger and more potent compounds, ultimately leading to the development of vemurafenib.

FBDD is a powerful tool in drug discovery and has the potential to help accelerate the development of new therapeutics. As technology and methods continue to advance, FBDD is likely to play an increasingly important role in the drug discovery process. Another advantage of FBDD is that it allows for a greater understanding of the molecular interactions between a drug and its target. By starting with small fragments and building up and gain insights into the specific interactions that contribute to a compound's binding affinity and selectivity. This information can be used to guide further optimization and can also aid in the development of drugs with improved properties.

FBDD also has the potential to facilitate the development of drugs for challenging targets, such as protein-protein interactions. These interactions are often difficult to target with traditional drug discovery methods, but FBDD can provide a starting point for the development of compounds that can disrupt these interactions.

Overall, FBDD represents a promising approach to drug discovery that can offer advantages over traditional methods. By starting with small fragments and building up, FBDD can help overcome challenges associated with traditional drug discovery and lead to the development of novel therapeutics. FBDD can also lead to the development of drugs with improved pharmacokinetic properties. Moreover, FBDD can be used to develop drugs that target multiple biological targets simultaneously. This approach, known as polypharmacology, can offer several advantages over single-target drugs, including increased efficacy, reduced resistance, and improved safety profiles.

Finally, FBDD can facilitate the development of personalized medicines. By using fragments that are specific to a particular genetic variation or disease subtype, FBDD can lead to the development of drugs that are tailored to individual patients. This approach can potentially improve treatment outcomes and reduce adverse effects.

Correspondence to: Mohan Krishna, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, West Bengal, India, E-mail: mohankrishna73@gmail.com

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