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Molecular Docking and Drug Repurposing Finding New Uses for Old Drugs

Raadan Konnai*

Laboratory of Infectious Diseases, Department of Disease Control, Graduate School of Veterinary Medicine, Japan

Abstract

This article explores the fascinating intersection of molecular docking and drug repurposing, showcasing how old drugs can find new life in alternative therapeutic applications. Drug repurposing, or repositioning, is gaining momentum as a cost-effective and time-efficient strategy to discover novel medical treatments. Molecular docking, a computational technique, plays a pivotal role in this process by enabling the study of ligand-receptor interactions and predicting binding affinities. Case studies highlight successful drug repurposing initiatives, emphasizing the role of molecular docking in uncovering these new applications. Challenges and prospects in the field are also discussed, underscoring the ongoing synergy between computational techniques and experimental validation. As the pharmaceutical industry evolves, the synergy between molecular docking and drug repurposing promises to expedite innovative therapy development, benefiting patients and reducing costs.

Keywords: Drug repurposing; Molecular docking; Computational drug discovery; Old drugs; New therapeutic applications; Ligand-receptor interactions; Binding afinity

Introduction

In the field of drug discovery, researchers are constantly on the lookout for new and innovative approaches to identify potential therapeutics. While the process of developing entirely new drugs is a time-consuming and expensive endeavor, drug repurposing, also known as repositioning, offers a promising alternative. This strategy involves the exploration of existing drugs, originally designed for one medical purpose, to discover new applications, often with the aid of molecular docking. In this article, we will delve into the world of molecular docking and how it plays a pivotal role in the process of repurposing old drugs for novel therapeutic uses [1].

The promise of drug repurposing

Drug repurposing is gaining traction in the pharmaceutical industry due to several compelling advantages. One of the most significant benefits is the potential for reduced development costs and timelines. Traditional drug development from scratch can take years and costs billions of dollars. In contrast, repurposing existing drugs can significantly expedite the process and save substantial resources.

Moreover, repurposing offers a higher likelihood of success. Since these drugs have already undergone extensive testing for safety and pharmacokinetics, their profiles are well-understood, reducing the risk associated with adverse effects. Additionally, repurposed drugs can often reach patients more quickly since they bypass many early-stage clinical trials [2,3].

Molecular docking

Molecular docking is a computational technique that plays a pivotal role in drug repurposing. It involves the study of the interaction between a drug molecule (the ligand) and its target protein (the receptor) at the atomic level. By simulating this interaction, researchers can predict the binding affinity and assess the potential of a drug to target a particular protein or pathway.

In the context of drug repurposing, molecular docking allows researchers to explore new therapeutic applications for existing drugs by virtually testing their interactions with different target proteins. This is accomplished by repurposing drugs for diseases or conditions that were not originally considered when they were first developed [4].

The steps in molecular docking for drug repurposing

Target identification: The first step is identifying a potential disease target, which could be a protein associated with a specific disease or condition.

Ligand preparation: In this step, the chemical structure of the old drug (the ligand) is optimized for docking simulations.

Receptor preparation: The 3D structure of the target protein (the receptor) is obtained, often through crystallography or homology modeling.

Docking simulations: Computational algorithms are used to predict how the ligand binds to the receptor. Various conformations and orientations are explored to assess binding affinity and efficacy.

Scoring and validation: Scoring functions are applied to rank the ligand-receptor interactions, and the results are validated through experimental assays [5].

Case studies in drug repurposing

Numerous successful drug repurposing stories highlight the effectiveness of molecular docking in this context. For instance, sildenafil, originally developed for cardiovascular conditions, was later repurposed as Viagra for erectile dysfunction. Thalidomide, once notorious for its teratogenic effects, found a new life in the treatment of multiple myeloma and leprosy.

***Corresponding author:** Raadan Konnai, Laboratory of Infectious Diseases, Department of Disease Control, Graduate School of Veterinary Medicine, Japan, E-mail: raadan.konnai@gmail.com

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Additionally, the antimalarial drug chloroquine was repurposed for the treatment of autoimmune diseases like rheumatoid arthritis and lupus. Such examples underscore the potential of drug repurposing and the role of molecular docking in uncovering these new applications [6,7].

Challenges and future prospects

While drug repurposing through molecular docking holds great promise, it is not without its challenges. Data integration, computational complexity, and the need for robust validation remain important issues. However, advances in artificial intelligence and machine learning are transforming molecular docking, making it more efficient and accurate.

As we move forward, the synergy between computational techniques like molecular docking and experimental validation will continue to uncover new uses for old drugs. The combination of these approaches will likely lead to the rapid development of innovative therapies, providing hope for patients and reducing the cost and time associated with bringing new treatments to market [8].

Discussion

Molecular docking is a computational technique used to predict the preferred orientation of one molecule (usually a ligand, which is a potential drug or bioactive molecule) when bound to a target molecule (usually a protein). It's a crucial step in the drug discovery process as it helps in understanding how a potential drug candidate interacts with its target at the molecular level. Here are some key points about molecular docking molecular docking can help identify potential binding sites on a target protein, which is essential for understanding how a drug might interact with the protein. Docking algorithms use scoring functions to estimate the binding affinity of a ligand to a target. These scores help researchers prioritize potential drug candidates. Docking is often used in virtual high-throughput screening, where a large number of compounds are evaluated computationally to identify those with the highest binding affinity.

Drug repurposing, also known as drug repositioning or drug reprofiling, is the process of finding new therapeutic uses for existing drugs that were originally developed for a different purpose. This approach offers several advantages. Repurposing existing drugs can significantly reduce the time and cost of drug development compared to developing new drugs from scratch. The safety profiles of repurposed drugs are often well-established, as they have already been used in humans for their original indications. Repurposed drugs typically have known pharmacokinetic and pharmacodynamic properties, making them easier to work with in terms of dosing and administration.Drug repurposing can be applied to a wide range of diseases, including rare and neglected diseases, where drug development might not be economically viable.

Molecular docking is often used in drug repurposing efforts to identify existing drugs that might interact with a new target. By virtually docking approved drugs against the protein associated with a new disease or condition, researchers can quickly identify potential candidates for further testing [9,10].

Conclusion

Molecular docking is a critical component of the drug repurposing process, allowing researchers to find new applications for existing drugs. This approach offers numerous advantages, including cost savings and a higher likelihood of success. As we continue to explore the vast landscape of existing drugs and their potential applications, molecular docking will remain an essential tool in the journey to find new uses for old drugs, ultimately benefiting patients and revolutionizing the field of medicine.

Conflict of Interest

None

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