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Review

Application of artificial intelligence in drug-target prediction

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Abstract: One of the most important problems in biomedicine is still drug development. AI-assisted drug development has emerged as a new trend, especially in anticipating drug-target relationships, as a result of the big data era and the quick growth of information technologies like artificial intelligence (AI). By efficiently extracting information from intricate biological data, properly modeling molecular interactions, and reliably forecasting possible drug-target outcomes, AI-driven models have become viable tools to tackle the problem of drug-target prediction. Convolutional neural networks (CNNs), graph convolutional networks (GCNs), transformers, and other sophisticated deep learning designs, as well as traditional machine learning (ML) and network-based approaches, are essential. Drug-target interaction prediction is a challenging task. AI-based DTI prediction can greatly increase speed, lower costs, and screen possible drug design choices prior to real tests thanks to the emergence of artificial intelligence (AI) techniques like machine learning and deep learning. Nevertheless, there are a number of issues with the use of AI techniques that must be resolved. This article examines several AI-based strategies and makes recommendations for potential future developments.

Keywords: Artificial intelligence (A.I.); drug-target prediction; drugs; machine learning

1. Introduction

There have historically been significant time and financial input costs associated with drug research and development. Moreover, forecasting experimental outcomes has shown to be difficult. The advent of artificial intelligence (AI) techniques in recent years, however, has presented a chance to lessen these problems. The wet experimental approach can be significantly enhanced by using AI for computational analysis and prediction, which will speed up drug research and development procedures and prevent needless costs. Finding and predicting drug-target interactions is crucial for both drug discovery and practical applications in biomedical fields, particularly drug repositioning. Predicting drug-protein interactions can help find new uses for already-approved medications, allow for the reevaluation of marketed medications, find new targets linked to other diseases, and speed up the investigation and development of new indications. It can help guide the design and development of new medications by forecasting how pharmaceuticals will interact with particular proteins[1-9].

Side effect prediction, where interactions between medications and proteins may result in drug side effects and adverse responses, is crucial for finding possible drug candidate compounds, speeding up the drug development process, and lowering costs and risks. Predicting drug-target interactions allows for the early detection of possible adverse effects, improving drug safety evaluation and monitoring. Additionally, by demonstrating how medications control biological processes to produce therapeutic benefits, these anticipated outcomes can aid researchers in their exploration and comprehension of the drug's mechanism of action. Finding customized treatments based on each person's unique genetic, phenotypic, and environmental traits could then lead to more accurate treatment outcomes. Artificial intelligence techniques can lower the cost of trial-and-error in following wet-lab work and boost efficiency, whether they determine how to screen out true positives as precisely as feasible or eliminate as many true negatives from the projected drug-target pairings as possible[1, 2, 6-8, 10, 11].

Drug-target interaction data encompasses a variety of information kinds, including drug and protein molecular structures, interaction specifics, clinical manifestations, drug side effects, and more. Of these, there are a lot more unknown interactions than recognized interactions between medications and targets. As a result, the imbalance between positive and negative data is the most frequent problem in this discipline, which makes it difficult to attain the best model performance. This certainly poses a significant obstacle. At the same time, the research of protein folding structures has gained more attention due to the integration and feature extraction of textual data as well as the introduction of

AlphaFold. The question of whether these three-dimensional structures might improve model predictions and how to optimize these possible advantages is brought up by their inclusion. The introduction of generative artificial intelligence (GAI) has created a new basis for creating drug molecules from the ground up, which has led to research and testing into the prerequisites for producing workable drug molecules with GAI. The viability of using quantum chemistry to explore enzyme catalysis reactions and optimize complicated structures at the particle level has also attracted interest and discussion in recent years. Lastly, the introduction of large-scale models facilitates quick contact and dialogue, which enables us to quickly arrive at a huge number of answers. Therefore, investigating how to incorporate drug discovery tasks while utilizing the potent reasoning powers of large language models (LLM) is a new frontier[12-20].

Predicting drug-target interactions is a critical use of AI and network pharmacology in drug development, as it is essential for determining possible therapeutic targets and comprehending pharmacological processes. Large-scale biological and chemical data can be analyzed by AI algorithms, especially deep learning and machine learning models, to determine which molecules are most likely to interact with particular targets. This feature lessens the need for conventional high-throughput screening techniques, which are frequently expensive and time-consuming, and speeds up the identification of viable drug candidates. This strategy is enhanced by network pharmacology, which offers a thorough understanding of the molecular networks underlying disease processes and highlights possible off-target effects and multitarget interactions. In order to overcome the long-standing problems of inefficiency and unpredictability in drug development, researchers can more precisely identify promising therapeutic targets and foresee potential side effects by combining AI's predictive capabilities with the systems-level insights of network pharmacology. By cutting down on time and expense, this collaboration not only improves the effectiveness of the drug discovery process but also offers fresh approaches to treating complicated illnesses by using multi-targeted tactics. In the end, this integration represents a significant step forward in the quest for precision medicine by helping to create safer, more individualized, and more successful medical therapies[1, 2, 21-24].

2. Association-based drug target prediction: In AI-driven drug development, association-based drug target prediction is essential. This method finds possible therapeutic targets by analyzing intricate biological networks and relationships between medications, targets, and illnesses using sophisticated machine learning algorithms and extensive biological data. This approach makes it easier to find new therapeutic targets and improves our comprehension of medication processes. Association-based predictions offer a strong framework for spotting important connections in the field of AI drug research, expediting the drug discovery procedure, and eventually assisting in the creation of more potent and specialized treatments[1].

3. Molecular collision-based drug target prediction: Drug target prediction models are based on the principles of molecular interactions and are mainly concerned with finding ligands that have the ability to either activate or inhibit particular proteins. These models aid in clarifying the molecular mechanisms of action by forecasting how medications will interact with their targets. They effectively find new medication candidates and offer insights into their molecular effects by utilizing computational methodologies[1].

4. Drug combination target prediction: Another essential element of AI-driven drug development is drug combination target prediction. This method finds synergistic interactions between several medications and their targets using sophisticated computational models. Drug combination target prediction helps identify intricate biological interactions that single-drug treatments could overlook by utilizing machine learning techniques and analyzing massive datasets. This approach improves the efficacy and safety profiles of treatment plans in addition to helping to comprehend the combined effects of medications. Predicting drug combination targets in the context of AI drug development has sped up the creation of new, more efficient treatment approaches, opening the door for precision and personalized medicine. These predictions are further improved by the incorporation of molecular collision models, which provide extensive insights into binding affinities and specificities by modeling the physical interactions between drug combinations and targets. Nevertheless, there are several drawbacks to using AI in medication research. Notwithstanding the potential demonstrated by these methods, there are still difficulties in guaranteeing the interpretability of AI models, particularly when addressing the complexity of biological systems. The fundamental understanding of how predictions are formed, which is essential for regulatory approval and clinical acceptance, may be obscured by the "black-box" nature of deep learning models. Furthermore, the performance of AI models is strongly impacted by the caliber and variety of the training data. Data biases may result in erroneous forecasts, which could have detrimental effects for medication development. This added complexity creates more difficulties when it comes to drug combination-target interactions. Although deep learning techniques like transformers and GCNs have demonstrated promise in simulating the combined effects of several medications, the possibility of unanticipated interactions and side effects is still a major worry. Furthermore, the availability of extensive training datasets that encompass the whole spectrum of potential drug interactions continues to restrict these models' capacity to forecast antagonistic and synergistic effects[1, 25, 26].

5. Conclusions and future perspectives: In AI-assisted medication development, interactions between the medicine and its target are essential. These approaches have greatly increased prediction accuracy and expanded the generalization capabilities of models by utilizing network-based models, conventional machine learning techniques, and

sophisticated deep learning techniques like CNNs, GCNs, and transformers. Understanding the intricate dynamics of medication combination-target interactions and detecting single drug-target interactions are two areas in which these developments are very helpful. They thereby speed up the drug discovery process and aid in the creation of more individualized and efficient treatments. The importance of these developments resides in their capacity to process and learn from enormous volumes of biological data, surpassing the constraints of conventional techniques that frequently find it difficult to handle the intricacy of molecular interactions.

Because multidrug interactions are more complicated, predicting drug combination-target interactions is more difficult. By simulating the combined effects of several medications on biological targets, deep learning techniques like CNNs, GCNs, and transformers have demonstrated potential in tackling these issues. The relational data included in pharmacological combinations is particularly well-represented and analyzed by GCNs, which offer insights into antagonistic and synergistic effects. Predicting how drug combinations may affect certain targets depends on transformers' capacity to process complex sequential data. In order to identify multitarget strategies and possible side effects, network-based models provide a comprehensive approach that is essential for comprehending the wider consequences of medication combinations inside biological systems. By mimicking the actual interactions between drug combinations and targets, the incorporation of molecular collision models improves these predictions even further and provides comprehensive information on binding affinities and specificities.

The combination of deep learning, network-based models, and conventional machine learning offers a strong foundation for improving drug discovery in spite of all the difficulties. These methods have the ability to completely transform the creation of customized treatments in addition to speeding up the identification of promising medication candidates. These technologies will probably have a greater influence on medication development as they advance, opening up new avenues for the treatment of complicated illnesses. To fully realize the potential of AI in drug research and clinical applications, it will be necessary to solve existing restrictions, such as assuring the ethical use of AI, improving data quality, and improving model interpretability.

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