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AI Models and Drug Discovery Within Pharmaceutical Drug Market

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Abstract

This literature review aims to highlight new drug discovery specifically in the United States, and introduce how artificial intelligence can be used to help reduce development time and costs.

Introduction

In the evolving landscape of healthcare, the pharmaceutical drug market plays a pivotal role in providing essential medications to individuals worldwide. This literature review aims to highlight new drug discovery specifically in the United States, and introduce how artificial intelligence can be used to help reduce development time and costs.

Drug Discovery

The drug discovery and development process is a lengthy, complex, and costly process. It is entrenched with a high degree of uncertainty that a drug will actually succeed. Developing a new drug from the original idea to the launch of a finished product is a complex process that can take 12–15 years and cost in excess of $1 billion.[1] The idea for a target can come from a variety of sources including academic and clinical research and from the commercial sector. A target can be a protein, DNA, or RNA that causes or contributes to a disease. Its validation consists of demonstrating that modulating the target has a therapeutic effect.[2] It may take many years to build up a body of supporting evidence before selecting a target for a costly drug discovery program. Once a target has been chosen, the pharmaceutical industry—and, more recently, some academic centers—have streamlined a number of early processes to identify molecules which possess suitable characteristics to make acceptable drugs. After the identification of a lead molecule that might produce the best-desired effects, lead optimization is done to consider it the preclinical candidate. Extensive amounts of testing must take place including in vitro, in vivo, preclinical, and clinical testing. It takes many years before testing begins on humans and even more to begin clinical trials. Arguably, the time and cost to develop a candidate drug are two of the largest challenges hindering companies from entering this process. By reducing the amount of time and overall cost of the R&D process, it could incentivize the creation of many new drugs and ultimately allow drug companies to reduce prices because of the decreased cost.

Artificial Intelligence

A potential innovation that can impact the drug market is artificial intelligence (AI), which is a field of study that combines computer science and large datasets in order to solve unique problems. Implementation of AI into the drug research and development process can reduce the cost, time, and amount of studies needed to get a drug created. Although this is a new application to this field, AI has already shown positive results in research, speeding up trials, and reducing the cost and risk related to preclinical and clinical trials.[3] Applying AI to the market can help provide a more efficient and targeted approach to drug discovery, thereby also increasing the likelihood of successful drug approvals.[4] The development of machine learning theory and the

accumulation of pharmacological data has allowed AI to impact various parts of the development process. Some of these areas include peptide synthesis, structure-based virtual screening, ligand-based virtual screening, toxicity prediction, drug monitoring and release, pharmacophore modeling, quantitative structure-activity relationship, drug repositioning, polypharmacology, and physiochemical activity.[5] One of the main applications of AI in drug design is the ability to assess specific molecular characteristics for fast *in silico* screening and identification of potential drugs with desired properties.[6] With these capabilities, AI has also been able to assist in the identification of lead molecules.[3]

There are numerous different algorithms that can be applied to large data sets to allow AI to interpret and display new insights into the data. Common machine learning algorithms include logistic regression (LR), naive Bayesian classification (NBC), k nearest neighbor (KNN), multiple linear regression (MLR), support vector machine (SVM), probabilistic neural network (PNN), binary kernel discrimination (BKD), linear discriminant analysis (LDA), random forest (RF), artificial neural network (ANN), partial least- squares (PLS), principal component analysis (PCA) and more.[3] These algorithms can be applied in a multitude of ways to provide researchers with various insight into their drug data. This can cause difficulty (especially for a non-specialist) to assess the usefulness and limitations of a particular method for the problem at hand.[6]

Research is being done on how effective AI is in the prediction of absorption, distribution, metabolism, excretion, and toxicology (ADMET) properties of lead drugs. The goal of evaluating ADMET properties is to accurately predict a candidate drug. AI can be beneficial in the deselection of compounds that have less favorable predicted ADMET properties and compounds to which various factions within the sponsor organization may feel strong attachment or decisional bias. AI has been found to improve the quality of hit and lead series and the probability of success of candidate compounds compared to what humans alone can do.[7] Humans still drive a majority of the research and development process though, as AI is not able to account for certain unamendable values such as enthalpy-entropy compensation, the chemistry of vicinal waters in receptors, multisite and multi-pose docking, and the picosecond timescale fluctuations of a receptor pocket.[7] While there are many uncertainties in AI modeling, AI should be used as a supplement to human expertise rather than substituting it. Confidence in AI decision quality should be made after careful evaluation of the methods, limitations of the algorithms being used, and the complexity of the model, and many other various factors.

It is also necessary to address that, within the drug design process, the number of parameters that may have influence on biological activity is typically high and relations may be strongly non-linear. With limited amounts of experimental data, the predictive ability of statistical learning systems may suffer from the "curse of dimensionality."[6] This could limit the application of AI to solely determine lead drug compounds. As of 2023 there have been no instances where AI or machine learning (ML) have solely determined a lead to candidate drug or later-stage development decisions.[7]

Utilization of AI enables the prioritization and optimization of lead compounds, reducing the need for extensive and costly animal testing. Personalized medicine approaches can be facilitated through AI algorithms that analyze real-world patient data, leading to more effective treatment outcomes and improved patient adherence.[4] Although to date the application of AI has been used as a supplement along with human oversight, the future holds promise for the improvement of AI models for use in an integrated manner within the drug development industry.

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Conclusion

Applying AI to the research and development of pharmaceutical drugs accelerates the drug discovery process and reduces development costs. This reduction in time and cost will not only help incentivize companies to develop new innovations, but also allow them to reduce the cost of prescription drugs and obtain more profit. Implementation of advanced AI models can help reduce the current financial burden prescription drug costs place on consumers within the US and other countries.

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