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REVIEW ARTICLE

Artificial Intelligence in Drug Discovery: A Review of AI Approaches for Target Identification

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ABSTRACT

Artificial Intelligence (AI) has become a revolutionary solution in drug discovery and development in aspects including high costs, long times, and high failure rates. This review describes the development and focuses on areas where AI has been used for target identification, lead optimization, design of new drugs from scratch and drug repurposing. Deep learning frameworks such as generative adversarial networks (GANs), variational autoencoders (VAEs), and explainable AI (XAI) approaches have been instrumental and comparative progress in enhancing the efficacy and specificity of drug discovery processes. AI has made advances in clinical trials, trial conduct, and participant selection, as well as enhanced patient-tailored therapies for personalized medicine. Issues such as data credibility, model explainability, and algorithmic biases are still present, and logical and social sciences' cooperation and code of conduct are needed. As such, this review aligns current developments with these challenges to demonstrate the possibilities of AI in revolutionizing pharma research and enhancing health solutions worldwide.

Keywords: Artificial Intelligence ▪ Machine Learning ▪ Drug Discovery ▪ Generative Models ▪ Clinical Trials ▪ Personalized Medicine

1. INTRODUCTION

Artificial Intelligence (AI) and Machine Learning (ML) are emerging innovative tools that can resolve the problems that have long plagued drug discovery. Notably, these technologies are revolutionizing significant steps in the drug discovery process, such as target identification and validation, lead identification and optimization, de novo design and drug repositioning. Sophisticated deep learning techniques, such as GANs and VAEs, are now allowing chemists to design new drugs with desirable pharmacological profiles. AI is also helpful in clinical trials and individualized medicine by selecting the most appropriate methodology for conducting the trials, better-selecting patient populations for clinical trials, and tailoring treatments to particular patients. This review endeavors to discuss the current developments, techniques, and uses of AI in drug discovery, focusing on its impact on redesigning pharmaceutical research and advancing healthcare delivery.

1.1 AI and ML in Drug Discovery

AI and ML are revolutionizing the first stages of drug discovery through the accurate identification of targets, the selection of leads and drug redeployment. Target identification is crucial in drug development. Since AI can parse through extensive biological and genomic data sets, it can quickly and accurately identify localized high-yield drug targets. Lead optimization, once carried out through several experimental cycles, is now boosted with AI algorithms that estimate molecular properties and improve compounds for increased effectiveness or reduced toxicity. The ability of AI to construct entirely novel structures in de novo drug design has also

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displayed the capability of creating novel and potentially useful drug-like material with favorable bioactivity. In addition, AI applications for drug repurposing reveal drug treatments, hence cutting costs and development time [1, 2].

1.2 Automated Generative Models for Drug Development

Conventional generative models such as GANs and VAEs have paved the way to de novo drug design. These models create new compounds by training from molecular data and synthesizing drug-like structures tailored to a particular disease's gene targets. For example, DDR1 kinase inhibitors and CDK20 inhibitors produced with generative frameworks prove that AI can design particular therapeutic agents. Reinforcement learning fine-tunes lead compounds by refining their structures. These models are revolutionizing drug discovery through fast and exhaustive searches in chemical space and the generation of candidates with specific pharmacological profiles [3].

1.3 Molecular Simulations and Computational Chemistry

Molecular simulations provide bottom-up information about interactions between drugs and proteins at the molecular level. Whereas AI uses predictions based on past data, molecular simulations apply physical laws to predict binding forces and develop better drugs. These simulations retain detailed structural and dynamic information on drug candidates, which is essential for optimizing efficacy and reducing side effects. When molecular simulations are combined with AI, the strengths of both techniques can be utilized, resulting in increased efficiency and precision.

1.4 AI in Clinical Trials and Personalized Medicine

AI contributes to clinical trials and individualized therapies by improving trial design, participant selection, and data analysis. Predictive models can identify suitable patient groups, monitor risks, and support adaptive trial protocols. AI also enhances personalized medicine by predicting patient responses, supporting real-time drug dosing, and evaluating drug combinations. Curated AI tools such as CURATE.AI support therapy optimization, while AI models predict beneficial interactions and help prevent adverse interactions. These innovations show that AI improves patient outcomes and makes healthcare more accurate and efficient [4, 5].

1.5 Optimization of Ethical and Technical Decisions

Despite rapid progress, several challenges affect the credibility of AI in drug discovery and development, including data refinement, algorithmic bias, and limited interpretability. Data is perhaps the most important aspect of prediction quality; credible data is complex, and erratic data remains an issue. In addition, the objectivity and fairness of AI algorithms should be addressed to establish trust between researchers and practitioners. These barriers require multi-disciplinary collaboration between AI specialists and pharmaceutical scientists to construct sound, open, and validated AI solutions [5].

AI and ML represent an exciting shift in the pharmaceutical industry's approach because they enable quicker, more efficient, and less expensive creation of new medications. Medical applications, molecular simulation, and AI-assisted clinical trial redesign have challenged old concepts and supported personalized patient treatment. However, issues of input data quality, model interpretability, and social impact should not be underestimated. With multi-disciplinary endeavors and sustained advancement in robust AI systems, the pharmaceutical sector has the potential to expand possibilities for new treatments.

2. LITERATURE REVIEW

The advancement of AI in drug discovery has challenged well-known paradigms in the pharmaceutical industry, including high costs, long development periods, and low success rates. Recent developments in ML and computing technology improve target identification, de novo drug design, and drug delivery systems. Technologies such as generative models and AI predictive tools have helped speed up the process and deliver personalized treatment plans. These innovations include cancer treatment, compatibility of traditional medicine, nanomedicine, and polypharmacology.

As outlined in [6], molecular property prediction is fundamental in drug discovery, leveraging graph neural networks to utilize molecular graph representations. While these models have succeeded across various applications, their decision-making process often lacks transparency. Concept whitening for graph neural networks creates interpretable models by identifying concepts and molecular structural components relevant to output predictions. Evaluations on benchmark datasets from MoleculeNet demonstrate that concept whitening layers enhance classification accuracy and interpretability.

As outlined in [7], AlphaFold's ability to predict protein structures for the entire human genome significantly advances artificial intelligence and structural biology. These predictions hold promise for structure-based drug design, particularly for targets lacking experimental structural data. By integrating AlphaFold into an AI-powered pipeline combining PandaOmics and Chemistry42 platforms, researchers identified a first-in-class small molecule hit for CDK20 with a Kd value of 8.9 ± 1.6 μM, requiring only 30 days and the synthesis of seven compounds. A subsequent iteration yielded a more potent molecule with a Kd value of 210.0 ± 42.4 nM.

As detailed in [8], integrating AI and ML has revolutionized drug discovery and highlighted the importance of transparency and interpretability in increasingly complex models. Explainable AI provides insights into predictions made by machine learning models. The review considers practical XAI approaches, discusses their use in target design and toxicity prediction, and addresses challenges and limitations.

Deep learning holds significant potential for advancing drug discovery and chemical biology, particularly in structure-based drug discovery [9]. By combining molecular representations, protein structure information, and ligand interaction learning, these approaches improve affinity prediction and binding elucidation. Other surveys categorize AI-driven drug discovery into representation, reasoning, and knowledge-driven sub-areas [1].

Computational omics technologies have accelerated natural product drug discovery by integrating AI for activity prediction and optimization [10]. AI in drug target identification and predictive modeling has been strengthened by AlphaFold2 and related protein prediction methods [11]. At the same time,

concerns remain regarding resource constraints, transparency, and the practical delivery of small-molecule drug discovery hits [12].

Recent applications also extend to colorectal cancer diagnosis and treatment optimization, drug delivery systems and personalized medicine, Traditional Chinese Medicine compatibility analysis, lung cancer clinical trials, and the integration of AI with molecular simulations [15, 16, 17]. Generative AI further accelerates molecular and drug design using GANs, VAEs, and reinforcement learning [18]. Comprehensive AI and ML frameworks are also being applied to polypharmacology, drug repurposing, combination therapy, and nanomedicine [19].

A summary of the paper's literature review is provided in Table 1, emphasizing specific works done on the use of AI in drug discovery and development.

Introducing AI in the drug discovery concept has already shown efficiency in making previous processes faster and more personalized regarding patient treatment outcomes. AI-driven technologies are revolutionizing pharmaceutical research, from efficient compound library generation to clinical trial optimization and integration of traditional and contemporary medicines. However, data quality, model interpretability, and ethical issues remain areas of concern before large-scale implementation.

3. DISCUSSION

AI is revolutionizing the drug discovery process because it provides solutions such as increased drug development efficiency, improved compound screening, and better predictive modeling. AI-based approaches have improved target identification, de novo drug design, clinical trial design, and personalized medicine by reducing development time and supporting more informed decisions.

3.1 AI-Based Drug Discovery and Development

AI and ML tools improve target identification, compound prioritization, and molecular optimization. Generative models can produce novel molecular structures, and predictive models can evaluate pharmacokinetic and toxicity properties before costly experiments. These capabilities help researchers explore chemical space more broadly and efficiently than traditional experimental cycles.

3.2 Artificial Intelligence in Clinical Trials and Precision Medicine

AI has positively impacted clinical trials through trial design improvement, better participant selection, and big data analysis. Real-time drug dosing and prediction of synergistic or toxic drug combinations can promote better therapeutic results. In personalized medicine, AI concepts involve finding biomarkers, selecting patient populations, and delivering treatment programs focused on the patient. Such innovations help minimize dangers and expenses and open the means of developing individualized and efficient health management systems [20].

3.3 Ethical and Technical Considerations

AI has many issues when applied to drug discovery technology. These include limited data quality, algorithmic bias, and lack of explainability. Lack of standard datasets and inadequate data refinement can cause variability in results, while complex AI models may introduce or hide bias. Solving these issues requires interdisciplinary programs that include AI researchers, drug discovery researchers, and development specialists, as well as clearer, valid, and ethical AI models [8].

3.4 Future Lines and Further Research Directions

The use of AI as a core technology in drug discovery means that the future of this area is a combined effort with other technologies such as molecular simulations and omics data. Integrating AI's large-scale prediction with molecule-by-molecule molecular simulations improves drug discovery pipelines. Integrating multiple omics data and multimodal artificial neural networks may also enhance understanding of pathology and drug interactions. Exploration of XAI methodologies and high-quality datasets will enhance model reliability and practical use in pharmaceutical research.

AI can effectively be applied in drug discovery, development, and personalized medicine, making processes faster and enhancing patient care quality. AI has already addressed target identification and clinical trials, representing notable pain points in earlier paradigms. Still, its potential is not widely realized due to ethical and technical challenges and the need for greater focus on data quality and interdisciplinary cooperation. By overcoming such challenges, AI can support improved, faster, more effective, and more accessible treatments.

4. CONCLUSION

Incorporating AI in drug discovery and development has been considered a paradigm shift. AI has dramatically impacted the drug development process by enabling the handling of large data sets, the creation of new molecular structures, and accurate computer modeling of biological interactions. Applications across the drug discovery value chain—from identification of the therapeutic target to de novo drug design, molecular modeling, pharmacokinetic and toxicity prediction, clinical trials, and precision medicine—show how AI has reinvented conventional methods, cutting time and expenses and enhancing treatment efficacy.

However, there are problems with extensive use of AI across the industry. Questions concerning data reliability and clarity of outcomes remain challenges that hinder the stability and proliferation of AI solutions. High-quality data is important because low-quality or inconsistent data leads to poor predictions, while the black-box problem associated with many AI algorithms raises concerns about fairness and ethical considerations. Meeting these barriers requires interpretable models and reliable datasets. Coordination between AI researchers, pharmacologists, and policymakers is also needed to guarantee that AI is used correctly in drug discovery.

The next step should be research on synergistic use of AI with other methodologies such as molecular simulation and multi-omics data analysis. Integrating these approaches can improve the ability of AI models to predict drug-target in-

Table 1. Summary of Literature Review

Reference	Focus Area	Key Contributions
[6]	Molecular property prediction using graph neural networks	Enhanced classification accuracy and interpretability using concept whitening layers.
[7]	AlphaFold in protein structure prediction and drug discovery	Identified CDK20 inhibitors, demonstrating rapid drug discovery capability.
[8]	Explainable AI (XAI) for enhanced drug discovery insights	Improved model transparency and interpretability in machine learning applications.
[9]	Deep learning for protein structure and ligand interactions	Highlighted structure-based drug discovery for affinity prediction and binding elucidation.
[1]	AI-driven sub-areas in drug discovery	Categorized AI advancements in drug representation, optimization, and reasoning.
[10]	Computational omics technologies for natural product drug discovery	Integrated AI for activity prediction and optimization in natural product discovery.
[11]	AI in drug target identification and predictive modeling	Highlighted protein prediction and AI-guided compound design.
[12]	Challenges in small-molecule drug discovery using AI	Addressed resource constraints and the need for transparency in drug development.
[13]	AI in colorectal cancer diagnosis and treatment optimization	Biomarker identification, treatment prediction, and early detection optimization.
[14]	AI in drug delivery systems and personalized medicine	Optimized drug formulation, screening, and real-world data analysis.
[15]	AI in Traditional Chinese Medicine compatibility analysis	Predicted TCM combinations and optimized compatibility ratios.
[16]	AI in lung cancer clinical trials and drug development	Streamlined trial designs, participant recruitment, and data analysis in lung cancer.
[17]	Integration of AI and molecular simulations in drug discovery	Combined AI top-down prediction with molecular simulation bottom-up analysis.
[18]	Generative AI (GenAI) for molecular and drug design	Accelerated de novo drug design using GANs, VAEs, and reinforcement learning.
[19]	Comprehensive AI applications in drug discovery processes	Developed innovative drugs such as DDR1 kinase inhibitors and enhanced polypharmacology.

teraction activity and disease pathways. The growth of XAI methodologies will also advance trust and usage across industry. By integrating other areas of study and enhancing these technologies, AI could meet the advanced needs of modern drug discovery.

With the progression of the pharmaceutical industry, AI remains one of the pinnacles of development that addresses inefficiencies, costs, and individual patient care. Addressing existing challenges will lead to the development of consistent and more accessible AI-assisted services that revolutionize drug development and treatment systems. Therefore, by adopting AI, the pharmaceutical industry can contribute positively to pressing global health needs by providing suitable solutions to society.

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