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Review Article

The role of Artificial Intelligence in drug discovery

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Abstract

The integration of artificial intelligence (AI) in drug discovery has revolutionized the field, offering unprecedented opportunities for accelerating the development of novel therapeutics. AI's adaptability and predictive capabilities have been successfully applied across various stages of the drug discovery process, including target identification, compound screening, and lead optimization. By leveraging machine learning algorithms and big data, researchers can expedite the discovery of promising compounds, reduce human workload, and improve the quality of life. This review provides a comprehensive overview of AI's role in drug discovery, highlighting its applications, advantages, and challenges. The current state of AI in drug discovery, its potential to transform the field, and the limitations that need to be addressed. Furthermore, explore the future directions of AI in drug discovery, including the need for high-quality data, standardization, and regulatory acceptance.

Keywords: Artificial intelligence, Drug discovery, Machine learning, Target identification

Introduction:

In recent years, several ideas related to artificial intelligence (AI) have been successfully applied in computer-assisted drug discovery [1]. The influence of artificial intelligence technologies on societal life has notably surged within the last decade [2]. Artificial intelligence (AI) showcases adaptability throughout numerous phases of the drug discovery process [3]. Both AI and machine learning technologies are instrumental in shaping this field [4].

Drug discovery has embraced emerging technologies like Utilizing data science, informatics, and AI can expedite the development of effective treatments, leading to reduced costs and fewer animal experiments. This shift is observable through rising enthusiasm from investors, industry experts, academic researchers, and policymakers [5]. Successful drug discovery process, and technologies related to machine learning and artificial intelligence are crucial in this area [6]. Technology's significance spans across all facets of life, including drug discovery endeavors [7]. The primary stage of drug discovery and development involves target identification and AI's expanding impact extends across numerous areas linked to drug discovery [8].

However, for widespread adoption by the medicinal chemistry community, it remains critical to develop AI models achieving high predictive performance while being explainable to end-users based on their knowledge and background [10]. AI operates using systems and software capable of learning from data to independently make informed judgments in pursuit of specific goals [11]. Since the 1960s, artificial intelligence (AI) has been used continuously in drug development at several stages, including target identification, lead optimization, and drug design [12,13]. Recent years have witnessed a rapid surge in using AI algorithms and big data in drug discovery, resulting in reduced human workload and considerable improvements in quality of life [14,15,16].

Advancements in AI technology significantly contribute to initial market analysis reports and accelerate research work in drug discovery [17,18]. The union of AI within the intricate landscape of drug discovery embodies an unprecedented convergence of technology and biology [19]. The process of discovering new drugs is time-consuming and costly, necessitating several steps to ensure the quality, safety, and potency of the marketed drug [20]. Potency against biological targets, selectivity against undesirable targets, and advantageous physicochemical and ADMET qualities are just a few of the requirements that clinical candidate compounds must meet in the drug discovery process [21]. Consequently, compound optimization remains a multidimensional challenge. The integration of artificial intelligence (AI) with novel

experimental technologies is anticipated to expedite, reduce costs, and enhance the efficacy of the search for new pharmaceuticals [22,23]. AI, in its diverse forms, is currently successfully applied in numerous domains and complex tasks, spanning robotics, speech translation, image analysis, logistics, and ongoing efforts in molecule design [24].

Drug Discovery involves a sequence encompassing candidate identification, synthesis, characterization, screening, and efficacy assays. Following successful testing, drug development ensues before clinical trials. This stage holds particular importance for the future, ensuring robust binding between the drug molecule and its target proteins or enzymes. Conventionally, discovering new drugs takes about 10-12 years, encompassing various research and development stages. The timeline flow diagram below illustrates the traditional drug discovery method. Each stage requires over a year, culminating in an overall drug approval timeframe of approximately 10-15 years [25, 26].

This study highlights the achievements in artificial intelligence, emphasizing its role in improving prior approaches to drug discovery [27].

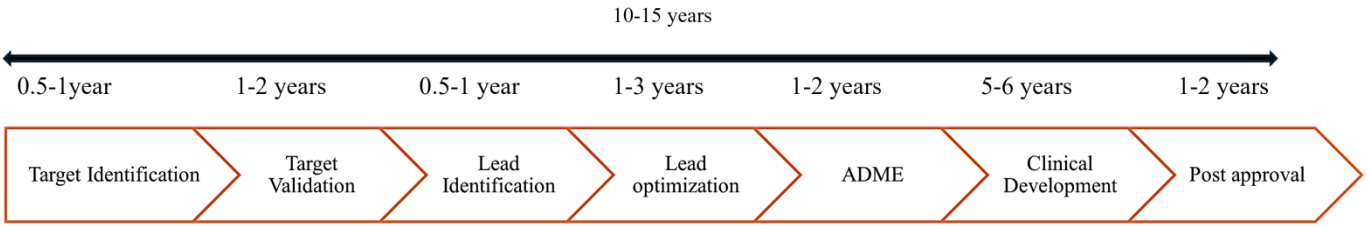

Figure 1: Traditional drug discovery timeline [28]

Artificial intelligence (AI):

Artificial intelligence (AI) is one of our era's swiftly advancing technologies. It represents a domain within computer science dedicated to creating intelligent systems [29].

Classification of AI: [30]

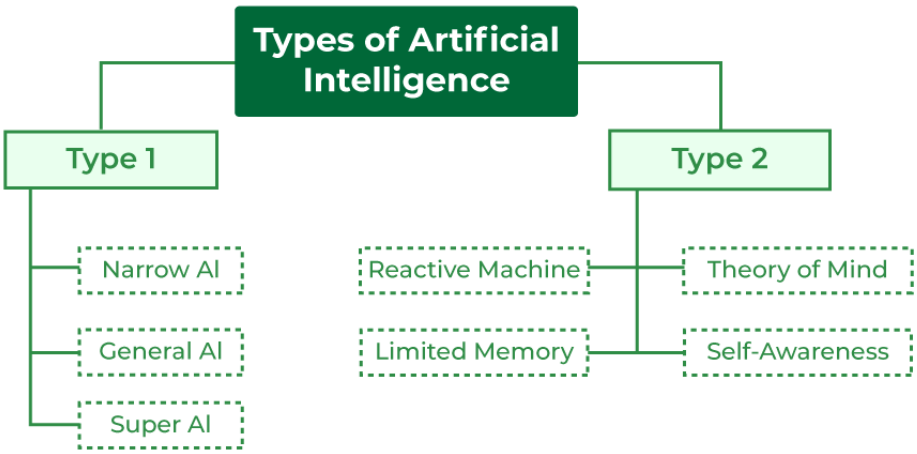

Figure 2: Types of Artificial Intelligence [30]

Artificial intelligence in drug discovery:

Artificial Intelligence (AI) has significantly impacted drug discovery [31], particularly in the challenging phase of finding new drugs, which has historically been the most arduous aspect since the outset of the drug discovery process [32]. The drug discovery and development process holds significant importance in identifying fresh therapeutic targets, screening potential lead compounds, and assessing drug efficacy and safety [33]. In the quest for anti-cancer drugs, the screening process often consumes considerable time. To expedite this process, Novartis utilized machine learning algorithms and images to predict potential subjects worth further exploration, capitalizing on the swift analytical capabilities of computers compared to traditional human analysis and laboratory tests [34]. This not only accelerates the discovery of promising compounds but also mitigates the labor costs linked to manually verifying each compound.

Cutting-edge intellectual property like the Jal Action Platform within leading biopharmaceutical companies holds the promise of enhancing health outcomes by enabling real-time data collection and integration in the quest for discoveries, often incorporating Wetware technology [35]. Also, after identifying potential targets drug ability, discovering drugs that interact with these therapeutic targets is crucial [36].

Given the complexity of treating concomitant diseases that might necessitate multiple drugs, predicting interactions between drug-target and drug-drug becomes essential to minimize the risks of increased side effects [37]. A transformative era in drug discovery research has been initiated by the development of AI, which has advanced from conventional trial-and-error or

hypothesis-driven methods to more rational, data-driven approaches [38]. AI and data-driven approaches, including AI are reshaping drug discovery processes [39].

Recent times have witnessed a renewed interest in incorporating deep learning into drug discovery, resulting in a remarkable upsurge in innovative modeling approaches and applications [40]. In drug discovery, AI techniques primarily fall into two categories: supervised learning and unsupervised learning. Unsupervised learning methods excel in exploratory data analysis by revealing concealed patterns within unlabeled data or facilitating data clustering [41]. The diverse spectrum of AI applications in drug discovery is depicted in the accompanying diagram. Despite its inherent advantages, AI grapples with significant data-related challenges such as managing issues related to data scale, expansion, diversity, and uncertainty [42].

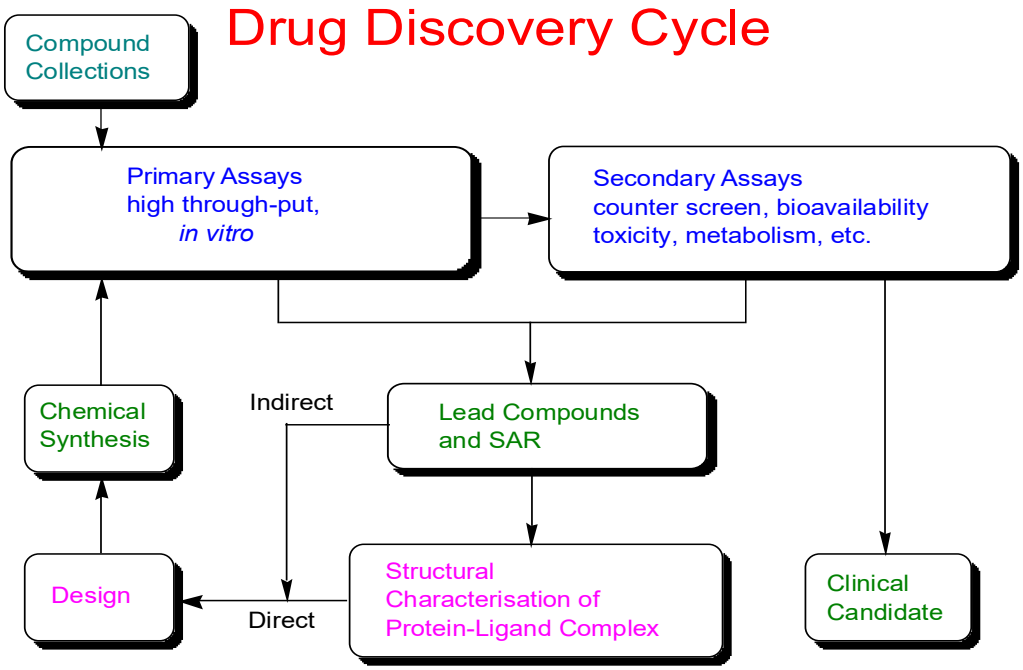

Figure 3: Drug discovery cycle [43].

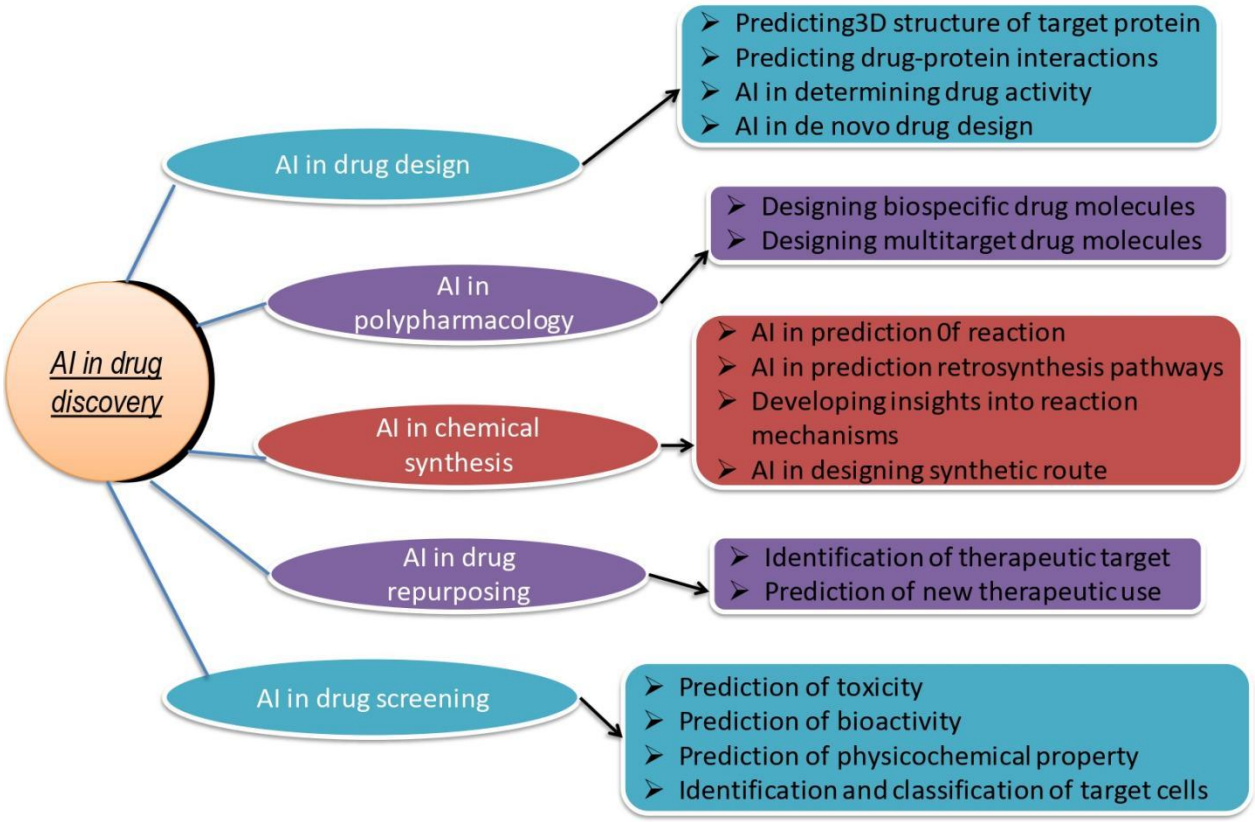

Figure 4: Role of artificial intelligence (AI) in drug discovery [44].

The process of drug discovery involves multiple intricate stages, generally categorized into four key phases: (i) target selection and validation; (ii) compound screening and lead optimization; (iii) preclinical studies; and (iv) clinical trials. Initially, identifying the target associated with a particular disease necessitates various evaluations, including cellular and genetic target assessments, genomic and proteomic analyses, as well as bioinformatic predictions [45]. The subsequent stage involves hit identification, where compounds are sourced from molecular libraries via techniques like combinatorial chemistry, high-throughput screening, and virtual screening. This phase employs a cyclic process of structure-activity studies, in silico analyses, and cellular functional tests to enhance the functional attributes of newly synthesized drug candidates [46].

Following this, in vivo studies, including pharmacokinetic assessments and toxicity tests, are conducted using animal models. Finally, the drug candidate, having passed through preclinical assessments, enters clinical trials involving three sequential phases: Phase I for testing drug safety with a small human cohort, Phase II for evaluating drug efficacy with a limited number of individuals affected by the targeted disease, and Phase III for conducting efficacy studies with a larger patient group. Approval and commercialization of the compound by regulatory bodies like the FDA follow if its safety and efficacy are confirmed during these clinical phases. Notably, the traditional drug discovery pipeline incurs an average cost of around 2.6 billion USD, with a timeline extending over 12 years [47].

Drug Discovery and Development Process: [48,49]

The drug discovery and development process include distinct stages:

1) Target selection and validation, a crucial phase involving the identification of disease-specific targets.
2) Compound screening and lead optimization, focused on refining drug leads sourced from molecular libraries to improve their desired properties.
3) Pre-clinical studies, comprising pharmacokinetic assessments and toxicity tests performed in animal models.
4) Clinical trials, where the potential drug candidate is administered to volunteers to assess any adverse effects.
5) Final approval of the drug for commercialization.

Advantages of AI In drug discovery: [51,52]

1. AI plays a crucial role in predicting environmental factors that can impact drug stability and shelf life, leading to improved formulation and durability of pharmaceuticals.
2. The implementation of AI significantly reduces the time and cost involved in medication development, making the entire research and development process more cost-effective.
3. AI contributes to error reduction and enhanced accuracy, utilizing intelligent robots for space exploration due to their robust construction and ability to withstand harsh conditions.
4. Industries such as mining and fuel exploration benefit from AI technology by rectifying human errors and enabling exploration in challenging environments, including oceanic studies.
5. AI facilitates everyday tasks; for instance, GPS aids in long commutes, while AI-powered androids predict user inputs and assist with tasks like spelling correction.
6. Modern businesses employ advanced AI systems, such as 'avatar' digital assistants, to reduce human intervention. These systems rely on logic and reason, avoiding the influence of human emotions, thereby enhancing judgment.
7. Medical applications of AI enable doctors to evaluate medication side effects and health risks, assisting in patient assessment and healthcare decisions without direct human intervention.

Disadvantages of AI in drug discovery: [52]

1. AI-equipped robots possess the capacity to mimic human thought processes while remaining detached from emotions, enabling more precise task execution without subjective judgment. However, AI lacks the capability to enhance human resources, as it cannot discern between diligent and inactive individuals based on experience.
2. Unlike AI technology, humans have the innate ability to exercise creativity and original thought processes that are beyond the current capabilities of artificial intelligence.
3. The widespread implementation of AI technology may lead to substantial unemployment, altering established work patterns and potentially stifling human workers creativity and innovation.
4. Implementing AI machines involves intricate design, maintenance, and repair processes that demand significant time and resources from the R&D sector. Regular software updates, machine reinstalls, and recovery procedures also contribute to the substantial time and financial investment in AI technology.

Application:

AI technology has found extensive application across the entirety of drug Research and Development (R&D), encompassing target identification, drug design, synthesis, and property evaluation. Undoubtedly, it has significantly reduced the drug R&D timeline and substantially reduced experimental costs when compared to conventional experimental procedures. Ongoing efforts by scientists to further integrate AI into various domains aim to foster the advancement of pharmaceutical sciences. AI's value in the drug discovery market is projected to grow significantly, with a compound annual growth rate of 40.8%, surging from 260 million USD globally in 2019 to an estimated 1.43 billion USD in 2024 [53].

1. Target identification in drug discovery:

In drug discovery, target identification aims at pinpointing molecules, commonly proteins, capable of altering disease states through modulation of their activity [54]. Machine learning algorithms possess the capability to analyze diverse datasets, including gene expression profiles, protein-protein interaction networks, and genomic and proteomic data. These algorithms aid in the identification of potential targets believed to play roles in disease pathways. Despite the vast human proteome comprising around 20,000 proteins, only about 3,000 have been recognized as potential therapeutic targets. Future advancements in knowledge might further augment our comprehension of proteins that could potentially serve as drug targets [55].

2. Virtual screening and optimization of compounds:

The pharmaceutical development research sector has witnessed a rising demand for in silico technologies and AI applications. This trend is expected to persist due to the necessity for precise forecasts of pharmacokinetics/ADMET (Absorption, Distribution, Metabolism, and Toxicity) concerning hit compounds. Evaluation of pharmacokinetics and toxicity remains crucial to prevent the potential failure of candidate drugs in later stages of drug development [56].

3. Pre-clinical and clinical development:

During this phase, a blend of favorable characteristics was pinpointed, prompting the initiation of clinical trials. Human volunteers serve as test subjects at this stage [57].

4. FDA approval and post-market analysis:

Natural Language Processing (NLP) finds applications in mining scientific literature to extract information regarding adverse effects, including drug toxicity or resistance, facilitating automated assessments essential for regulatory (FDA) approval or patent applications [58]. Additionally, NLP-based sentiment analysis techniques can suggest drugs [59]. Furthermore, machine learning-based systems capable of predicting potential product sales assist pharmaceutical companies in optimizing their business resources. The FDA acknowledges the emerging issues with 3D printing and is actively researching to comprehensively understand the technology [60].

5. Preclinical studies, focusing on pharmacology, pharmacokinetics, and toxicology, rely on understanding a drug's physicochemical properties and ADMET characteristics [61].

6. Pediatric patients unique needs for safe drug products and adherence require specific considerations in drug design due to limited clinical trials for pediatric applications [62].

7. Compound solid preparations, composed of multiple parts with varying amounts of medicine, undergo processes like pulverization, mixing, screening, drying, and molding to form solid medicine preparations [63].

8. AI assists in developing complex formulations, predicting physicochemical parameters, and optimizing drug stability, solubility, and viscosity for injectable and biologics, enhancing formulation development [64].

Challenges and limitations of AI in drug discovery:

The term "Artificial intelligence in drug discovery" may imply successful implementation of AI in early drug discovery stages [65]. However, while AI-driven drug discovery holds significant promise, it faces several persistent challenges and limitations. The interpretability of deep learning models poses a concern as comprehending the reasoning behind model predictions is vital to establish trust in these predictions. Furthermore, issues related to data quality, standardization, ethical implications, and regulatory acceptance of AI-driven drug discovery methods are crucial aspects that demand attention [66].

Despite the existing potential benefits of AI in drug discovery, various challenges and limitations need careful consideration [67]. A primary challenge involves the availability of appropriate data [68]. AI-driven approaches typically necessitate a vast amount of data for effective training [69].

Inefficient data integration presents another issue arising from the divergence between datasets containing raw data, processed data, metadata, or candidate data [70].

Successful applications of AI in drug discovery:

Over the past few years, multiple reviews have highlighted the increasing importance of AI in drug discovery. Therefore, this specific review intends to focus on a range of noteworthy studies that demonstrate the practical influence of AI in small-molecule drug discovery [71].

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