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A review on Artificial Intelligence in drug discovery and designing

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***Abstract*—Artificial intelligence (AI) is quickly becoming an important part of modern drug discovery and design, helping scientists tackle many of the problems associated with traditional pharmaceutical research. Developing new medicines has always been a long, expensive, and risky process, often relying on repeated trial-and-error experiments. Today, advances in AI—particularly in machine learning, deep learning, natural language processing, reinforcement learning, and quantum computing—are changing this approach by making drug discovery faster, more accurate, and more efficient at every stage. This review explains how AI is being applied throughout the drug discovery pipeline, from identifying disease-related targets and predicting molecular properties to designing new drug candidates, studying protein structures, planning chemical synthesis routes, and improving clinical trial design. Special focus is given to deep learning techniques such as convolutional, recurrent, and graph neural networks, which have proven highly effective in predicting drug–target interactions, toxicity risks, and pharmacokinetic behavior. Breakthrough technologies like AlphaFold have further transformed structure-based drug design by allowing researchers to accurately predict the three-dimensional shapes of proteins directly from their amino acid sequences.**

The article also explores newer applications of AI in areas such as clinical trial optimization, personalized medicine, self-driving laboratories powered by robotics, nanomedicine, and nanorobotics. These innovations enable automated experiments, more precise drug delivery, improved patient selection, and quicker, data-driven decisions, all of which help shorten development timelines. However, despite its strong potential, AI adoption in drug discovery still faces challenges, including issues with data quality, bias, limited transparency of models, high computational requirements, and regulatory approval.Overall, AI is not designed to replace human expertise but to work alongside scientists and clinicians, supporting better insight, creativity, and decision-making. With ongoing collaboration among researchers, healthcare professionals, regulators, and industry partners—and as ethical and regulatory frameworks continue to develop—AI is expected to play an increasingly important role in creating safer, more effective, and more personalized therapies, ultimately improving patient care and global health outcomes.

***Index Terms*—Artificial Intelligence (AI), Drug Discovery, Drug Design, Machine Learning, Deep Learning, De Novo Drug Design.**

I. INTRODUCTION

Artificial intelligence (AI) has become a familiar part of everyday life, with major advances in areas such as image and speech recognition, natural language processing, and other data-driven technologies [1,]. Some of the most striking achievements of AI are seen in computers outperforming world-class human players in complex games. A well-known example is IBM's Deep Blue, which defeated chess champion Garry Kasparov in 1997 using hard-coded rules and brute-force computing. In contrast, Alpha Go learned the game by playing against itself and later defeated the world's top Go players, marking a significant shift in how AI systems learn and improve [2].

AI is commonly defined as intelligence demonstrated by machines, especially when they display abilities typically associated with human thinking, such as learning, reasoning, and problem-solving. It includes a wide range of technologies, most notably machine learning, which is used to discover patterns in data and make predictions. Among these approaches, artificial neural networks—particularly deep neural networks (DNNs) and recurrent neural networks (RNNs)—have been key drivers of recent progress in AI[3].In pharmaceutical research, AI gained widespread attention when deep learning models began to outperform traditional methods in predicting molecular properties and biological activities. This was clearly demonstrated in challenges such as the Merck Kaggle competition and the NIH Tox21 challenge , where deep neural networks achieved higher predictive accuracy than standard machine learning approaches. Since then, AI applications in early drug discovery have expanded rapidly, moving beyond property prediction to areas such as de novo design of chemical compounds and peptides, as well as automated synthesis planning.

Over the past few years, numerous review articles have offered comprehensive introductions to the use of AI in drug discovery.In this article, we focus on recent developments in artificial intelligence related to property and activity prediction, de novo molecular design, and retrosynthetic strategies[4]

Artificial Intelligence (AI) is a broad field of computer science focused on creating machines that can carry out tasks usually performed by humans. These tasks include learning from experience, recognizing patterns, understanding language, solving problems, and making decisions. AI systems work by using algorithms, large datasets, and strong computing power to mimic certain ways humans think and learn. Today, AI is widely used in areas such as language translation, robotics, self-driving cars, and medical diagnosis. As AI continues to evolve, it has also raised important questions about ethics, employment, and its long-term effects on society.

Researchers often classify AI systems based on their abilities and range of functions. Narrow AI, also called Weak AI, is designed to perform specific tasks, such as voice recognition or image classification. General AI, or Strong AI, refers to systems that could perform many different tasks at a level comparable to human intelligence. Beyond this is Super intelligence, which describes AI that could potentially outperform humans in all areas of thinking and problem-solving . Each of these categories reflects a different level of development and influence on human life.

AI already has a strong presence in many industries, including healthcare, finance, and transportation. In these fields, it is used for tasks such as personalized recommendations, detecting fraud, and assisting with medical diagnoses . As the demand for AI-driven solutions continues to increase, ongoing advancements in AI technology suggest a future where AI plays an important role in tackling complex global challenges and supporting human capabilities [5]

Machine learning has become an important tool in computer-assisted drug discovery, helping researchers identify and design new medicines more efficiently .In recent years, deep learning approaches—especially artificial neural networks with multiple hidden layers—have attracted growing attention. This is largely because they can automatically learn meaningful patterns from raw data and capture complex, nonlinear relationships between inputs and outputs . These abilities make deep learning a strong complement to traditional machine learning methods, which typically rely on manually created molecular descriptors.

Although the adoption of deep learning in drug discovery was initially slow, interest in this area has increased rapidly over the past few years . This growing attention has led to a surge in new modeling strategies and real-world applications . As a result, many fields within the chemical sciences are already benefiting from continuous advances in deep learning technologies . This opinion article explores, through selected examples, the key reasons why deep learning methods have been so successful and, in some cases, have outperformed existing approaches in chemoinformatics.

Drug discovery

recent years, artificial intelligence (AI) has attracted increasing attention in medicinal chemistry for its potential to reshape the pharmaceutical industry . Drug discovery—the process of finding and developing new medicines—is inherently complex and time-consuming, and it has traditionally depended on labor-intensive methods such as high-throughput screening and trial-and-error testing. Today, however, AI technologies, including machine learning (ML) and natural language processing, enable researchers to analyze large amounts of data more quickly and accurately, helping to streamline and improve the drug discovery process [6].

Recent research has shown that deep learning (DL) models can successfully predict the potency of medicinal compounds with high accuracy . In addition, AI-based methods have been used to predict the toxicity of potential drug candidates, allowing safety concerns to be identified at earlier stages of development. Together, these advances demonstrate how AI can significantly improve both the speed and effectiveness of drug discovery.Despite these encouraging developments, the use of AI to design new bioactive compounds is not without challenges. Further research is needed to better understand the limitations of these technologies, and ethical considerations must be carefully addressed. Even so, AI is widely expected to play an increasingly important role in the development of new drugs and therapies in the years ahead [7].

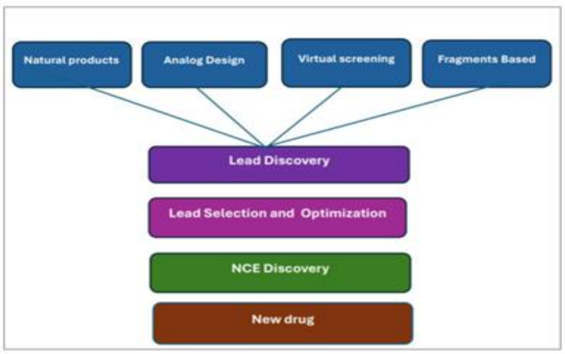

Fig 1. Drug Discovery

Drug design

that you want to designate with a certain style, then select Artificial intelligence (AI) is playing an increasingly important role in speeding up drug development by improving the way promising lead compounds are identified during the drug design process. By analyzing large numbers of molecular structures and predicting how strongly they might bind to biological targets, AI helps move potential drugs more efficiently from early ideas to clinical testing [8]. At the heart of drug design is the challenge of finding small molecules that meet several key requirements, including strong therapeutic effects, acceptable safety profiles, suitable chemical and biological properties, and enough novelty to support intellectual property protection and commercial success .

While computational tools have already transformed drug discovery, traditional methods still face limitations such as long processing times, high computational costs, and variable reliability . AI helps overcome these challenges by improving the speed, accuracy, and overall effectiveness of computational approaches used in drug development .

Because many diseases are linked to problems in protein function, understanding protein structure is essential for modern drug discovery. Structural drug design focuses on identifying small molecules that can interact specifically with target proteins. In the past, predicting the three-dimensional (3D) structure of proteins was often slow, expensive, and prone to error. Recent advances in AI—especially in deep learning and automated feature extraction—have greatly improved this process. These techniques allow for more accurate prediction of protein structures and protein–protein interactions, deepening our understanding of how protein sequences determine structure and function.

The long-term goal is to use deep learning to reliably predict complete 3D protein structures, enabling detailed studies of protein–protein interactions and supporting more effective structure-based drug design . This integration of AI into drug discovery represents a major step forward, offering faster development timelines, reduced costs, and improved success rates.

Accurate prediction of protein 3D structures is a critical step in structure-based drug discovery , and AI methods—particularly machine learning and deep learning—play a central role in meeting this challenge . AI-based protein structure prediction depends on large and diverse datasets of protein sequences and known structures. By learning from these data, AI models can identify complex patterns that link amino acid sequences to their corresponding 3D structures [9].

Deep learning models have demonstrated a strong ability to capture subtle patterns in protein data by analyzing amino acid properties, structural motifs, and evolutionary relationships. Using this information, AI systems can predict protein structures directly from sequence data. A major breakthrough in this field is AlphaFold, developed by Google DeepMind. AlphaFold predicts 3D protein structures by estimating distances between nearby amino acids and the angles of peptide bonds. In a recent evaluation, AlphaFold successfully predicted 25 out of 43 protein structures, highlighting its potential for structure-based drug development .

Although traditional experimental techniques for determining protein structures remain highly accurate, they are often expensive and time-consuming. AI provides a faster and more cost-effective alternative by generating reliable 3D protein models directly from sequence data . This capability allows researchers to design drugs that are more precisely matched to their target proteins, enabling earlier evaluation of drug effectiveness and safety.

In addition, AI methods such as molecular dynamics (MD) simulations can use predicted protein and drug structures from databases like the Protein Data Bank (PDB) and DrugBank to study how protein–drug complexes behave over time. These simulations provide insights into their stability, movement, shape, and binding strength, helping researchers better understand molecular interactions . AI has also shown strong potential in modeling complex biological relationships through graph-based machine learning approaches. By representing chemical systems as graphs—with atoms as nodes and bonds as connections—these methods can capture detailed relationships among drugs, diseases, protein–protein interactions, and side effects, supporting drug repurposing and more accurate prediction of treatment responses. More quickly and accurately, helping to streamline and improve the drug discovery process .

AI in Clinical Trial Design

Designing a clinical trial is a crucial step in bringing new medicines to patients. This process involves deciding how many clinical events are needed to obtain reliable results, estimating how often these events may occur in the target population, determining how many patients should be enrolled, and defining how long participants need to be followed. Throughout the trial, patients are carefully monitored until the required number of events is reached. Developing a new drug is a lengthy and expensive journey, often taking 10 to 15 years and costing between USD 1.5 and 2.0 billion [10]. A significant portion of this time and expense is spent on clinical trials, which alone can take 6–7 years and require substantial financial investment.

Although clinical trials are essential for evaluating the safety and effectiveness of new drugs in humans, their success rates remain very low. Only about one out of every ten compounds that enter clinical trials ultimately receives regulatory approval, resulting in major financial losses for the pharmaceutical industry. These failures can occur for many reasons, including poor patient selection, unmet technological needs, and inadequate infrastructure . In addition, preclinical activities such as compound discovery, testing, and regulatory preparation account for nearly half of total research and development costs.

Recruiting the right patients is one of the most difficult and time-consuming aspects of clinical trials, often accounting for almost one-third of the total trial duration. Inappropriate patient selection alone is responsible for approximately 86% of trial failures. These long timelines, high costs, and low success rates highlight the urgent need for new technologies that can make clinical trials more efficient, reduce development time, and lower overall costs.

The growing availability of digital medical data has made artificial intelligence (AI) a promising tool for transforming clinical trial design and execution. AI has the potential to improve many aspects of clinical trials, ultimately speeding up the development and delivery of new therapies [11]. For example, AI algorithms can rapidly screen thousands of compounds by modeling how drug molecules interact with biological targets, significantly reducing the time and resources needed in the early stages of drug discovery.

AI also plays an important role in drug discovery and biotechnology through the simulation of bio molecular structures using physics-based methods such as molecular dynamics (MD). These simulations examine three-dimensional structures of proteins and drugs obtained from databases like the Protein Data Bank (PDB) and DrugBank, as well as structures predicted by advanced AI models such as AlphaFold2 . MD simulations allow researchers to explore the stability, movement, shape, and binding behavior of protein–drug complexes over time. By applying advanced data analysis techniques, including deep learning, scientists can gain valuable insights into molecular interactions, disease mechanisms, and drug responses or resistance.

AI techniques in drug discovery

Drug discovery has long been a challenging, time-consuming, and costly process, often requiring more than a decade and billions of dollars to bring a single medicine to patients. As biomedical data continues to grow rapidly and the demand for faster, more efficient drug development increases, artificial intelligence (AI) has become an important tool in modern pharmaceutical research. Today, AI is helping transform every step of the drug discovery process, from identifying biological targets and designing new molecules to conducting preclinical studies and improving clinical trial design.

Several AI techniques are playing a key role in this transformation, including machine learning (ML), deep learning (DL), natural language processing (NLP), reinforcement learning (RL), and quantum computing (QC). These methods allow researchers to analyze enormous datasets, uncover complex patterns, and make accurate predictions that would be extremely difficult or time-consuming using traditional approaches. Together, these AI technologies are changing how new drugs are discovered and developed, with the potential to reduce costs, shorten development timelines, and improve overall success rates.

Machine Learning

Machine learning (ML) has become an essential tool in modern drug discovery because of its ability to analyze complex, high-dimensional biological data. ML algorithms learn from existing datasets to identify patterns and make predictions about new compounds. Supervised learning methods, such as support vector machines (SVMs) and random forests, are commonly used to predict drug-target interactions, toxicity profiles, and pharmacokinetic properties (ADMET). For example, ML models can estimate the likelihood of a compound binding to a specific protein, enabling virtual screening of large chemical libraries without the need for costly laboratory experiments [12].

Unsupervised learning techniques, like clustering, help group compounds with similar properties or discover entirely new chemical scaffolds. Reinforcement learning, though less commonly used, is increasingly applied to optimize chemical synthesis pathways. When combined with high-throughput screening and omics data, ML accelerates target identification and validation, allowing researchers to focus on the most promising drug candidates early in the development process.

Deep Learning

Deep learning (DL), a specialized branch of machine learning, uses neural networks with multiple layers to capture complex, non-linear relationships in data. In drug discovery, DL has transformed how molecular information and biological structures are analyzed. Convolutional Neural Networks (CNNs) are particularly effective at interpreting spatial data, such as 3D molecular structures and protein-ligand binding sites, allowing accurate prediction of binding affinities and drug-target interactions. Recurrent Neural Networks (RNNs) and their variants are well-suited for sequential data, such as chemical sequences (SMILES) or protein sequences, helping detect patterns that traditional models might miss. More recently, Graph Neural Networks (GNNs) have gained attention because they represent molecules as graphs, directly modeling atoms and chemical bonds [13].

DL has also been instrumental in the success of AlphaFold, which predicts protein structures with remarkable accuracy, speeding up target characterization. However, deep learning models require substantial computational resources and large labeled datasets, which can limit their use. Techniques like transfer learning and data augmentation are helping to overcome these challenges.

Natural Language Processing (NLP)

Natural Language Processing (NLP) has become a vital tool for extracting meaningful insights from the vast and ever-growing body of biomedical information, including research articles, patents, and clinical trial reports. With scientific publications increasing at an exponential rate, manual curation is no longer practical. NLP automates the extraction of key information, enabling researchers to quickly identify chemical compounds, biological targets, and experimental results.

Techniques such as named entity recognition (NER) can detect drug names, genes, and diseases, while relation extraction models uncover interactions and biological pathways, producing structured data that can be used for further analysis. NLP also supports the creation of knowledge graphs that link data from different sources, helping to identify opportunities for drug repurposing or discovering new biomarkers[14].

Recent advances in transformer-based models, such as BERT and its biomedical adaptations BioBERT and SciBERT, have greatly improved the understanding of domain-specific scientific language . NLP can also summarize research findings and assist in designing clinical trial protocols, making decision-making in drug development faster and more efficient. Challenges remain, such as handling ambiguous terminology and conflicting data, but continuous improvements in model architectures and training datasets are enhancing the accuracy and utility of NLP. Overall, NLP unlocks hidden knowledge in textual data, bridging information gaps and accelerating innovation in drug discovery.

Reinforcement Learning (RL)

Reinforcement learning (RL) is an AI approach in which an agent learns to make decisions by interacting with an environment, aiming to maximize cumulative rewards over time. Unlike supervised learning, RL does not rely on labeled datasets; instead, the agent learns optimal strategies through trial and error, guided by feedback in the form of rewards or penalties.

In drug discovery, RL has become a powerful tool for optimizing complex, multi-step processes such as molecular design, synthesis planning, and the fine-tuning of pharmacological properties. RL frameworks treat molecule design or chemical modification as a sequence of decisions. The agent iteratively adjusts molecular structures and receives feedback based on criteria like drug-likeness, binding affinity, toxicity, or synthetic feasibility . This iterative exploration allows RL models to discover innovative compounds that satisfy multiple constraints at once, often outperforming traditional rule-based methods[15].

RL can also be combined with generative models, such as Variational Autoencoders (VAEs) or Generative Adversarial Networks (GANs), to guide molecule generation toward desired properties using customized reward functions. Beyond molecule design, RL is applied to optimize synthetic pathways, helping researchers identify efficient chemical reaction routes to produce target compounds, thereby reducing time and cost in the lab.

Quantum Computing (QC)

Quantum computing (QC) represents a transformative leap in computational power, using principles like superposition and entanglement to perform certain calculations far faster than classical computers. In drug discovery, QC is especially promising because molecular interactions are inherently quantum, and many chemical simulations are too complex for traditional computing methods to handle accurately.

Quantum algorithms can simulate molecular electronic structures and protein folding with remarkable precision, providing detailed insights into how drugs interact with their targets at the atomic level. This capability can greatly improve predictions of binding affinities, reaction pathways, and other physicochemical properties, accelerating lead optimization and reducing the reliance on costly experimental testing[16].

At present, quantum hardware is still in the noisy intermediate-scale quantum (NISQ) era, which limits the size and complexity of problems that can be practically addressed. Nonetheless, hybrid quantum-classical methods—such as the Variational Quantum Eigensolver (VQE) and the Quantum Approximate Optimization Algorithm (QAOA)—are being explored to perform small-molecule simulations and solve optimization problems relevant to drug discovery[15].

Challenges and Limitations of AI in Drug

Artificial intelligence (AI) has the potential to revolutionize drug discovery, but several key challenges must be addressed before its full benefits can be realized.

One major hurdle is access to high-quality, well-curated, and diverse datasets. AI models rely heavily on large, reliable datasets, and their performance depends directly on the data used during training. Yet collecting such data can be difficult due to strict privacy regulations, fragmented ownership across institutions, and limited mechanisms for sharing information. For smaller research labs and startups, gathering and managing these datasets can be both costly and time-consuming. Collaborative initiatives and data-sharing frameworks are therefore essential to ensure access to comprehensive and representative datasets.

Another challenge is data bias and limited generalizability. AI models trained on biased or incomplete data may produce inaccurate or misleading predictions. Bias can arise from unequal representation of populations in clinical trials, regional differences in healthcare practices, or variations in experimental protocols. Overfitting—when a model performs well on training data but poorly on new, unseen data—is another common issue. This can lead to the selection of ineffective drug candidates or a higher number of false positives. Researchers address these challenges using bias-mitigation strategies, such as the Synthetic Minority Oversampling Technique (SMOTE), which generates synthetic data for underrepresented groups to balance datasets. While no method completely eliminates bias, careful dataset selection, preprocessing, and bias-correction can significantly improve AI predictions in drug discovery.

Computational demands also present a significant challenge, especially for deep learning models. Training and deploying these models requires substantial computing power, advanced hardware, and specialized expertise, which can be a barrier for academic labs and smaller pharmaceutical companies. Many organizations address this by using cloud-based computing platforms or partnering with AI technology providers, making advanced computational tools more accessible while reducing costs.

Finally, regulatory approval and model validation remain critical obstacles. For AI-driven tools to be widely adopted in drug discovery, their predictions must be transparent, reproducible, and scientifically validated. Regulatory agencies require clear evidence demonstrating the safety, reliability, and effectiveness of AI-generated insights. Building trust in these systems will require close collaboration among regulators, pharmaceutical companies, and AI researchers to develop standardized evaluation frameworks and validation guidelines.

Pharmaceutical Market of AI

To reduce the high costs and risks of failure associated with traditional drug discovery, pharmaceutical companies are increasingly turning to artificial intelligence (AI). The AI market in the pharmaceutical sector has grown rapidly, rising from around USD 200 million in 2015 to USD 700 million in 2018, and it is expected to reach USD 5 billion by 2024 [16]. This represents a projected growth rate of approximately 40% from 2017 to 2024, highlighting AI's potential to transform both the pharmaceutical and healthcare industries.

Many pharmaceutical companies are actively investing in AI and forming partnerships with technology firms to develop innovative healthcare solutions. A notable example is the collaboration between DeepMind Technologies, a subsidiary of Google, and the Royal Free London NHS Foundation Trust, aimed at improving the management of acute kidney injury. Figure 4 provides an overview of key pharmaceutical companies and AI players driving innovation in this rapidly evolving space [17].

AI in De Novo Drug Design

De novo drug design involves creating completely new drug-like molecules without relying on existing compounds or known templates . This strategy is especially powerful because the number of possible drug-like molecules is enormous—estimated to range from 10^{60} to 10^{100}. Exploring such a vast chemical space using traditional methods is extremely difficult and time-consuming. In recent years, artificial intelligence (AI), particularly machine learning and deep learning, has emerged as a key enabler for tackling this challenge and is transforming how new therapeutic molecules are discovered

Traditional de novo design approaches often face major limitations, including complex synthesis pathways and uncertainty in predicting the biological activity of newly generated molecules. AI helps overcome these challenges by learning from large chemical and biological datasets to identify patterns that connect molecular structures with their pharmacological effects [18]. As a result, AI-driven models can suggest new molecules that are more likely to be biologically active, safe, and synthetically accessible.

Generative AI models have been especially successful in de novo drug design. Methods such as variational autoencoders (VAEs) and generative adversarial networks (GANs) learn the underlying patterns of molecular representations and use this knowledge to generate entirely new chemical structures with desired properties [19]. For instance, Gómez-Bombarelli and colleagues developed a VAE-based approach that maps chemical structures into a continuous latent space, making it possible to efficiently generate and optimize novel molecules by navigating this space .

Deep reinforcement learning (DRL) has also attracted growing interest in this field. In DRL-based approaches, molecule generation is treated as a step-by-step decision-making process. A notable example is the Reinforcement Learning for Structural Evolution (RLSE) framework, which combines generative and predictive deep neural networks. The generative model proposes new molecular structures, while the predictive model evaluates their properties and provides feedback. Using this strategy, researchers have successfully generated molecules targeting receptors such as retinoid X and PPAR, demonstrating promising therapeutic potential.

The Impact of AI on the Drug Discovery Process and Potential Cost

Artificial intelligence (AI) is playing an increasingly important role in drug discovery, particularly by enabling the design of entirely new compounds with specific biological properties. Traditional drug development often focuses on modifying existing molecules, a process that can be slow, costly, and limited in its ability to explore new chemical space. In contrast, AI-based methods can rapidly generate novel molecules that are optimized for key characteristics such as potency, solubility, and safety, making the early stages of drug discovery faster and more efficient.

Recent studies have demonstrated that deep learning (DL) models trained on large datasets of known drugs and their properties can successfully propose new therapeutic candidates with improved biological activity and favorable physicochemical properties [20]. These findings highlight how AI can reduce reliance on time-consuming trial-and-error approaches and significantly accelerate early-stage drug design.

A major milestone in AI-driven drug discovery is the development of AlphaFold by DeepMind, a powerful system capable of predicting the three-dimensional structures of proteins directly from their amino acid sequences . By providing highly accurate protein structures, AlphaFold has greatly enhanced our understanding of molecular interactions and biological mechanisms. This breakthrough is expected to have a lasting impact on structure-based drug discovery and personalized medicine, as it enables researchers to design drugs that more precisely target disease-related proteins.

In addition, machine learning (ML) techniques are increasingly being integrated with molecular dynamics (MD) simulations in de novo drug design to improve both efficiency and predictive accuracy. ML models can quickly identify promising drug candidates, while MD simulations offer detailed insights into the stability, motion, and binding behavior of protein–drug complexes. The growing use of interpretable machine learning (IML) and deep learning approaches further helps researchers understand and trust AI predictions, supporting more informed and rational decision-making throughout the drug development process.

AI in the life cycle of pharmaceutical product

Artificial intelligence (AI) has the potential to enhance pharmaceutical product development at every stage, from early laboratory research to clinical application at the patient's bedside. In the early phases, AI supports rational drug design by helping researchers identify and optimize promising drug candidates more efficiently . Throughout development, AI also enables better decision-making, including selecting the most suitable therapies for individual patients, thereby supporting personalized and precision medicine. Additionally, AI can efficiently manage and analyze the large volumes of clinical data generated during trials, using these insights to guide and improve future drug development efforts [21].

Beyond research and development, AI is increasingly being used for commercial and strategic decision-making within the pharmaceutical industry. One example is E-VAI, an AI-driven analytical and decision-support platform developed by Eularis. By combining machine learning algorithms with a user-friendly interface, E-VAI generates strategic insights based on competitor behavior, key stakeholders, and market share data. This enables marketing and business leaders to better allocate resources, anticipate market trends, address declining sales, and identify high-impact investment opportunities.

Robotics artificial intelligence in pharmacology

Hand- On'' to "Self- Driving'' discovery

Robotics and artificial intelligence (AI) are fundamentally changing how drugs are discovered and developed. Processes that once depended on intensive manual labor are now evolving into automated, data-driven systems that can operate continuously. In this new approach, AI systems plan experiments, while robotic platforms carry them out day and night without interruption.

By following well-defined experimental protocols, these AI-driven systems can repeatedly design experiments, test ideas, learn from results, and improve their predictions. Each experiment adds new knowledge, allowing the system to become more accurate over time. This continuous feedback loop not only accelerates drug discovery but also improves reproducibility and the overall quality of the data, reducing reliance on trial-and-error methods.

Figure 8 shows how AI and robotics come together in a "self-driving" drug discovery laboratory. Within the design–make–test–analyze (DMTA) cycle, AI proposes the most promising experiments, and robotic systems perform them automatically. The resulting data are analyzed and fed back into the AI models, which then refine their predictions and plan the next steps. Over multiple cycles, this closed-loop process produces reliable, audit-ready datasets and helps identify optimized drug candidates more efficiently.

In this self-reinforcing DMTA workflow, every cycle builds on the last. Experimental results continuously improve the AI's ability to design better molecules and make smarter decisions. The ultimate goal is to generate high-quality data, clear documentation, and drug candidates that are ready to advance toward clinical development.

Self-driving laboratories represent a major step beyond traditional high-throughput screening and automated chemistry. They push drug discovery toward full autonomy, where machines not only conduct experiments but also decide which experiments to perform next(22,23) As emerging initiatives show, the integration of AI and robotics is already beginning to transform pharmacology and accelerate the development of new medicines.

AI application in various stages of drug discovery:

Diseases and therapy selection

Recent improvements in computing technology have greatly accelerated the adoption of artificial intelligence (AI) in health care. Today, AI is being used in many areas, such as identifying diseases, analyzing medical images, classifying medical conditions, and assessing how drugs are used and what treatments are most effective. With its growing potential to improve the quality and efficiency of health-care services, this section examines how AI is reshaping medical diagnosis and supporting more informed and personalized treatment decisions.

Diseases and health care :

In the past ten years, rapid improvements in computing technology have significantly changed how diseases are diagnosed, with many studies showing how AI is being used in fields such as dermatology, tuberculosis, Alzheimer's disease, diabetes, hypertension, and cancer. AI can play an important role in improving many areas of health-care management, such as helping doctors make more accurate diagnoses, analyzing medical images, enhancing communication between patients and health-care providers, and improving the day-to-day operations of hospitals and nursing homes. It can also support population health by considering social and environmental factors and by analyzing real-world health data. As of March 30, 2023, most experts agree that AI is best seen as a tool that assists health-care professionals, rather than one that will replace them anytime soon.(25).

Image based AI

AI tools that work with medical images are increasingly being used in fields like radiology, pathology, and dermatology. Pathology, in particular, is shifting toward a digital approach, where tissue samples and laboratory slides are scanned and stored as digital images. These images can then be used to train AI systems, making the analysis faster, more consistent, and more accurate. Computational pathology aims to make disease diagnosis and classification more accurate and reliable by minimizing errors. At the same time, it helps researchers identify new biomarkers more quickly, gain deeper insights into how diseases develop, and strengthen research efforts in areas such as animal studies and toxicology.

AI in nanotechnology-based products

Research in nanotechnology and personalized medicine is changing quickly as new tools and technologies emerge. The combination of automation and artificial intelligence (AI) is enabling scientists to design and fine-tune therapeutic nanoparticles that can be tailored to specific cell types and individual patients. AI is already playing a major role in applications like nanomedicine and nanobots, where it helps improve the precision, effectiveness, and overall success of treatments.

Nanomedicine

Nanomedicine involves applying nanotechnology to medicine to help diagnose diseases more accurately, deliver treatments more effectively, and improve overall health care outcomes. Nanomedicine is transforming both the treatment of diseases and the monitoring of their progression. By delivering drugs directly to targeted areas in the body and keeping them active for longer, it has greatly improved the care of complex and life-threatening conditions. In recent years, clinical nanomedicine has achieved impressive milestones, with numerous studies and approvals demonstrating its promise. For instance, the PLGA-Docetaxel complex has been explored for treating breast cancer, while clinical trials are underway for the Spherical Nucleic Acid (SNA) platform targeting glioblastoma. Other approved therapies include PEGylated liposomal doxorubicin (DOXIL) and albumin-bound paclitaxel (Abraxane), which are now used to treat pancreatic, lung, and breast cancers.(24)

Nanorobots

Nanorobots are incredibly small, man-made machines that can detect their surroundings, move, and carry out tasks at the nanoscale with precision and control. Unlike traditional drug delivery methods, these tiny robots can target specific areas, perform multiple tasks at once, and offer greater control and efficiency. Recent advances in nanotechnology have sparked growing interest in creating nanorobots powered by internal or external energy sources, equipped with sensors, and enhanced with artificial intelligence.

Nanorobots hold great potential for detecting harmful substances, as well as for therapeutic and diagnostic purposes. Artificial intelligence (AI) can help direct their movement and behavior. Coordinating multiple nanorobots requires advanced swarm intelligence algorithms, which are inspired by the way insects, birds, and animals work together without a central leader. One such approach, called the Swarm Intelligence Method,(25) is specifically designed to control nanorobots. The three most common types of swarm intelligence algorithms are ant colony optimization (ACO), artificial bee colony (ABC), and particle swarm optimization (PSO).

Particle Swarm Optimization (PSO) has been improved into an advanced technique called Directed Particle Swarm Optimization (DPSO). This method is designed to steer nanorobots directly toward cancerous areas in the body. Studies have shown that DPSO can guide nanorobots to tumor sites quickly and efficiently.

In one study, DPSO was compared with four other optimization methods to evaluate its performance. The results revealed that DPSO performed better than the other approaches, especially in minimizing the time required to deploy nanorobots. This speed makes it possible to deliver a large number of nanorobots to the cancer site in a short period, increasing the effectiveness of targeted cancer treatment.

Additionally, Artificial Neural Networks (ANNs) are increasingly being used to predict how nanorobots behave when combined with biosensors and transducers. This approach is considered highly promising for detecting tumor cells and improving targeted drug delivery. By enhancing accuracy and responsiveness, these intelligent systems contribute to more effective and precise nanorobot-based cancer therapies.

Fig 2 . Application of nanotechnology

II. CONCLUSION

Artificial intelligence has become a major force in modern drug discovery and development. From identifying potential drug targets and designing new molecules to improving clinical trials, nanotechnology, and personalized medicine, AI is changing how new treatments are created and delivered. By analyzing large and complex sets of biological, chemical, and clinical data, AI reduces the need for slow trial-and-error methods, shortens development timelines, lowers costs, and increases the likelihood of success. Recent progress in machine learning, deep learning, natural language processing, reinforcement learning, and quantum computing has greatly improved the prediction of molecular behavior, protein structures, drug–target interactions, and possible toxicity. Breakthroughs such as AlphaFold have revolutionized structure-based drug design, while generative and reinforcement learning models have made it easier to explore vast chemical spaces during de novo drug discovery.

At the same time, combining AI with robotics and self-driving laboratories has led to automated systems that learn from each experiment and continuously improve, moving drug development closer to full automation. Beyond discovery and design, AI is also playing an important role in clinical trial planning, healthcare decision-making, nanomedicine, and nanorobotics. In these areas, intelligent systems support earlier disease detection and more precise drug delivery. Despite these advances, challenges such as data quality, transparency of AI models, high computational demands, bias, and regulatory approval still limit widespread use. Addressing these issues will require strong collaboration among researchers, industry, and regulatory bodies.

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