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ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY: REVOLUTIONIZING PHARMACEUTICAL RESEARCH

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ABSTRACT

The pharmaceutical industry is undergoing a transformative shift with the integration of Artificial Intelligence (AI) in drug discovery. AI technologies, including machine learning, deep learning, and natural language processing, are revolutionizing traditional methods by accelerating the identification of potential drug candidates, optimizing chemical structures, and predicting drug properties with unprecedented accuracy. The adoption of AI in pharmaceutical R&D has facilitated groundbreaking collaborations, enhanced the development of novel therapies, and significantly reduced attrition rates. This review explores the history, current landscape, and future prospects of AI in drug discovery, highlighting its applications in target identification, virtual screening, de novo drug design, and predictive modeling. While challenges and limitations exist, the strategic integration of AI with traditional approaches is poised to transform the pharmaceutical industry, ultimately enhancing patient care and global healthcare outcomes.

KEYWORDS: Artificial Intelligence (AI), Machine Learning (ML), Deep Learning (DL), Natural Language Processing (NLP).

INTRODUCTION

Artificial intelligence (AI) has emerged as a transformative tool in drug discovery, offering innovative solutions to the challenges of time, cost, and efficiency in pharmaceutical research. By simulating human intelligence processes, AI enables data acquisition, rule-based analysis, and self-correction, revolutionizing traditional methods. Techniques such as

machine learning (ML), deep learning (DL), and natural language processing (NLP) allow researchers to predict drug properties, identify potential candidates, and optimize chemical structures with unprecedented accuracy.[1-2]

Despite challenges such as ethical considerations and data biases, AI significantly accelerates the drug development pipeline, improving precision and reducing attrition rates. Its growing adoption in pharmaceutical R&D has facilitated groundbreaking collaborations and enhanced the development of novel therapies.[3]

HISTORY

Artificial Intelligence in

Artificial Intelligence (AI) in medicine involves the use of advanced algorithms, techniques, and computer systems to analyze medical data, assist in decision-making, and perform tasks traditionally handled by healthcare professionals. AI aims to enhance the accuracy, efficiency, and effectiveness of medical diagnosis, treatment, and patient care by leveraging technologies such as machine learning (ML) and natural language processing (NLP).[4]

AI applications in healthcare span diverse areas, including medical imaging, drug discovery, personalized treatment planning, disease prediction, electronic health record (HER) management, and patient monitoring. By analyzing vast datasets and medical literature, AI systems help healthcare professionals make informed decisions, detect patterns, and predict outcomes, improving patient care and treatment success rates.[2]

History Development

1950s to 1970s: Early Innovations

The foundation of AI began with machines capable of mimicking human tasks. Key milestones included the development of the industrial robot arm Unimate (1961), the chatbot Eliza (1964), and the mobile robot Shakey (1966), which processed complex commands. In medicine, digital innovations like PubMed and clinical informatics systems laid the groundwork for AIM's future growth, although early adoption in healthcare was slow.

1970s to 2000s: Challenges and Progress

This period, often referred to as the "AI Winter," was marked by reduced funding and interest in AI, with significant advancements limited. Notable developments included the creation of medical decision-support systems such as MYCIN (for infectious diseases) and DXplain (for

differential diagnosis). Collaboration among pioneers helped sustain progress, such as the establishment of the Research Resource on Computers in Biomedicine and the first AIM workshop in 1975.

2000 to 2020: Seminal Advancements

AI in medicine gained momentum with advancements like IBM Watson's DeepQA system, which demonstrated capabilities in evidence-based decision-making. Virtual assistants like Siri (2011) and Alexa (2014) introduced meaningful conversational AI. Pharmabot (2015) and Mandy (2017) expanded AI applications to medication education and patient intake processes. The rise of DL, powered by improved computing and larger datasets, enabled advanced models like convolutional neural networks (CNNs) for image analysis, transforming medical imaging diagnostics.[4]

AI IN PHARMA MARKET

Artificial Intelligence (AI) in the pharmaceutical industry refers to the application of automated algorithms to tasks typically requiring human intelligence. AI solutions in pharma can analyze vast datasets, such as disease patterns, and help identify the most effective medication formulations for specific conditions. The AI in pharma market is divided by technology (such as natural language processing, deep learning, and context-aware processing), by drug type (including small and large molecules), and by application (including diagnosis, clinical trials, drug discovery, research and development, and epidemic prediction).

Market Size and Growth

The AI in pharma market has seen substantial growth in recent years. From $1.58 billion in 2023, it is expected to expand to $2.06 billion in 2024, marking a compound annual growth rate (CAGR) of 30.4%. This growth is attributed to the increasing use of AI for cost-effective drug discovery and its rising implementation in fields like radiology.

Forecast for Market Growth

Looking ahead, the AI in pharma market is projected to experience significant growth, reaching $5.62 billion by 2028 with a CAGR of 28.5%. Key factors driving this expansion include the adoption of cloud-based services, increasing healthcare spending, and greater government support for AI advancements. Notable trends in the forecast period include the rise of generative AI, AI integration in drug screening, AI tools for pharmaceutical

applications, and growing strategic collaborations and investments in the development of new product solutions.[5]

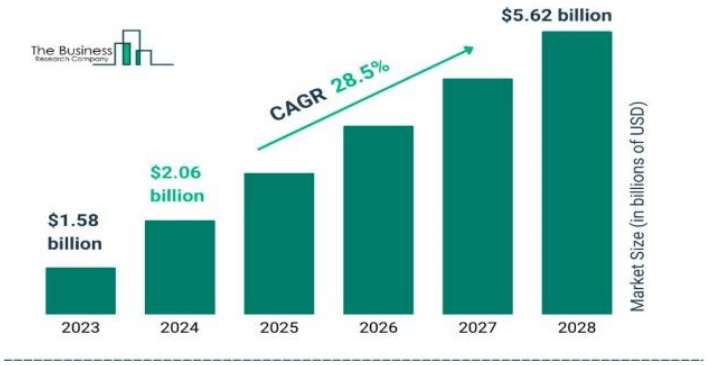

Figure 1: AI in Pharma Global Market Report 2024)

AI TECH. PHARMACEUTICS

The concept of artificial intelligence (AI) is continually advancing, driven by the development of cutting-edge technologies like machine learning (ML), deep learning (DL), and natural language processing (NLP), which aim to replicate human intelligence with increasing precision.

Machine learning (ML)

Machine Learning (ML) is a subset of Artificial Intelligence (AI) that empowers machines to learn from experience and make decisions without being explicitly programmed. ML achieves this through the use of algorithms and neural networks, enabling automated analysis and prediction.

ML algorithms are broadly categorized into the following types

Supervised Learning

Supervised learning involves training a model on a labeled dataset where the outcomes are predefined. The algorithm learns patterns and relationships between the input data and the corresponding outputs, making it suitable for tasks such as classification and regression.

Applications in Pharmaceuticals

Drug Discovery and Design: Predicts the properties of new drug candidates by analyzing molecular features and desired outcomes.

Predictive Maintenance and Quality Control: Identifies equipment failures or quality deviations in manufacturing processes.

Disease Diagnosis and Prognosis: Helps diagnose diseases and predict treatment outcomes based on medical data.

Adverse Event Detection: Identifies safety signals by classifying patterns in adverse event reports.

Predictive Modeling for Clinical Trials: Predicts patient responses and optimizes trial designs using historical trial data.[7]

Techniques

Naïve Bayes, K-Nearest Neighbors, Support Vector Machines, Random Forests, Linear Regression, Ensemble Learning, etc.[7]

Unsupervised Learning

Unsupervised learning uses unlabeled data to uncover patterns and relationships. In drug discovery, it is applied to identify new material classes and explore chemical spaces for potential drug candidates.

Techniques like k-means group data based on similarity, aiding in identifying compounds with similar properties. Hierarchical clustering organizes compounds into a hierarchy, providing insights at different levels of detail.

Methods like principal component analysis (PCA) and t-SNE reduce data complexity while retaining key features. These techniques help visualize high-dimensional data, revealing hidden patterns and trends in drug discovery research.[3]

Applications in Pharmaceuticals

Clustering: Groups data points (e.g., gene expression profiles, patient data) to identify subgroups for target identification or patient stratification.

Dimensionality Reduction: Simplifies high-dimensional data while preserving critical information using techniques like Principal Component Analysis (PCA) and t-SNE.

Anomaly Detection: Detects rare patterns in data for adverse event identification or safety concerns.

Association Rule Mining: Discovers relationships (e.g., drug-drug interactions or co-occurrence patterns) to aid pharmacovigilance.

Topic Modeling: Extracts themes from large text datasets (e.g., clinical trial reports or literature) for trend analysis and competitive intelligence.

Techniques: K-Means, Hierarchical Clustering, Isolation Forest, Apriori Algorithm, Pearson Correlation, etc.[7]

Reinforcements Learning (RL)

Reinforcement learning involves training algorithms through interactions with their environment. The model receives rewards for favorable outcomes, reinforcing positive behaviors over time.[6]

ML's Impact on Pharmaceuticals and Drug Discovery.

Machine learning (ML) is revolutionizing various aspects of pharmaceuticals and drug discovery. It accelerates drug discovery through virtual screening, molecular modeling, and predictive analytics, helping to identify and optimize drug candidates quickly. In precision medicine, ML analyzes patient data, including genomics and clinical records, to enable personalized treatments and develop biomarkers for diagnosis and prognosis. ML also plays a significant role in drug repurposing by identifying new therapeutic uses for existing drugs, offering a faster and more cost-effective approach. Additionally, ML optimizes drug formulations, predicting release kinetics and enhancing delivery systems to improve efficacy and patient compliance. In clinical trials, ML aids patient recruitment, optimizes trial protocols, and enables real-time data analysis for adaptive trial designs. It also supports safety and compliance by identifying potential adverse events, ensuring regulatory adherence, and enhancing pharmacovigilance. ML further contributes to supply chain optimization by predicting demand, optimizing production schedules, and improving quality control. Pharmaceutical companies like Pfizer, Novartis, and Roche are leveraging ML to enhance drug formulations, predict drug interactions, and personalize treatments, demonstrating how ML is transforming the landscape of drug discovery and development.[7]

Deep Learning

Deep learning, a subset of machine learning, is designed to process and analyze data through multiple interconnected layers of algorithms. These layers aim to extract high-level abstractions from data by employing complex structures and nonlinear transformations. Unlike shallow learning models like Support Vector Machines and Logistic Regression, which were prominent in the 1990s and featured minimal or no hidden layers, deep learning is built on multi-layer neural networks. These networks enable the progressive learning of data features, where the output of one layer serves as the input for the next, allowing for the identification of intricate patterns and relationships within data.[8]

Deep learning frameworks, such as Convolutional Neural Networks (CNNs), Restricted Boltzmann Machines, Deep Belief Networks, and Generative Adversarial Networks, have revolutionized areas ranging from image recognition to natural language processing. The release of tools like OpenAI's ChatGPT in late 2022 highlighted the capabilities of deep learning for a wider audience. Unlike earlier innovations like DALL-E and Stable Diffusion, ChatGPT introduced deep learning technology to the public through an accessible API, allowing users to experience firsthand its potential in generating human-like responses based on extensive datasets.[9]

Deep learning Techniques

Deep learning (DL) techniques have emerged as a cornerstone of modern machine learning (ML) applications, playing a pivotal role in areas such as spam detection, video recommendation systems, image classification, and multimedia retrieval. Among the numerous ML approaches, DL has become one of the most widely adopted due to its superior performance in handling complex tasks. This rapid advancement in DL can be attributed to the ever-changing nature of data acquisition and significant improvements in hardware technologies.

Building upon the foundation of traditional neural networks, DL surpasses their capabilities by utilizing advanced transformations and graph-based technologies to construct multi-layer learning models (Kim et al., 2021). With its transformative approach, DL has reshaped how complex problems are addressed. The flexibility and adaptability of deep learning models enable them to solve intricate challenges that conventional methods cannot effectively handle. The following section explores various deep learning models and their impact across diverse domains.[10]

Convolutional Neural Networks (CNNs)

Convolutional Neural Networks (CNNs or ConvNets) are primarily utilized in computer vision and image processing tasks. They excel in identifying patterns and features within images and videos, enabling applications such as object detection, image recognition, face recognition, and pattern analysis. CNNs rely on principles of linear algebra, particularly matrix operations, to analyze patterns in visual data.

A CNN is a specialized type of neural network, consisting of multiple layers: an input layer, one or more hidden layers, and an output layer. Each node within these layers is interconnected, with assigned weights and thresholds. When the output of a node surpasses the set threshold, the node becomes active, transmitting data to the next layer. Otherwise, the data does not progress further through the network.

The architecture of a CNN typically includes three primary layers: convolutional layers, pooling layers, and fully connected (FC) layers. In more complex applications, CNNs can comprise thousands of layers, with each layer building upon the patterns identified by the previous ones. Through iterative convolutions—repeated transformations and refinements of the input data—CNNs detect intricate patterns and relationships. Initial layers focus on simple features like edges and colors, while subsequent layers recognize larger components or shapes, ultimately enabling the identification of the target object.

CNNs outperform traditional neural networks in handling image, audio, or speech data. Before CNNs were developed, manual feature extraction methods were labor-intensive and time-consuming. CNNs now offer a scalable, automated approach to tasks like image classification and object recognition, processing high-dimensional data effectively. They also allow data sharing across layers, improving efficiency and reducing complexity. While pooling layers may lead to some information loss, the overall benefits of CNNs—such as reduced complexity, minimized risk of overfitting, and enhanced performance—often outweigh this drawback.

Despite their advantages, CNNs come with challenges. They are computationally intensive, requiring significant time, resources, and advanced graphical processing units (GPUs). Additionally, deploying CNNs demands skilled professionals with expertise in multiple domains. The configuration and optimization of CNNs, including hyperparameter tuning, require rigorous testing and careful calibration to ensure optimal performance.

Recurrent Neural Networks (RNNs)

Recurrent Neural Networks (RNNs) are widely used in applications involving sequential or time-series data, such as natural language processing (NLP), speech recognition, language translation, and image captioning. They are also effective in tasks like stock market predictions and sales forecasting. Popular tools like Siri, Google Translate, and voice search often integrate RNN-based functionalities.

A key feature of RNNs is their use of feedback loops, allowing them to retain "memory" of previous inputs to influence current outputs. Unlike traditional neural networks that treat inputs as independent, RNN outputs depend on prior elements in the sequence. However, standard RNNs can only process past data and cannot account for future inputs in their predictions.

RNNs share parameters across layers, with weights adjusted using backpropagation through time (BPTT). This technique calculates errors for sequence data by summing errors at each time step, differentiating it from traditional backpropagation. RNNs also enable versatile outputs, producing one-to-many, many-to-one, or many-to-many results depending on the application.

One common variant, the Long Short-Term Memory (LSTM) network, outperforms standard RNNs by addressing longer-term dependencies.

Despite their strengths, RNNs face challenges such as vanishing and exploding gradients. Vanishing gradients occur when weight updates become too small, halting learning, while exploding gradients cause unstable models with excessively large weights. Solutions include simplifying models by reducing hidden layers. Additionally, RNNs often require lengthy training times and are complex to optimize, especially with large datasets and multiple layers.

Autoencoders and Variational Autoencoders (VAEs)

Autoencoders, a type of neural network, process unlabeled data by encoding it into a compressed format and then reconstructing it back to its original form. While basic autoencoders are useful for tasks like denoising images, Variational Autoencoders (VAEs) extend this capability by not only reconstructing data but also generating variations of the original input. This innovation played a crucial role in the development of deep generative models, laying the foundation for generative AI.

VAEs have been instrumental in creating realistic images and speech, sparking advancements in technologies like Generative Adversarial Networks (GANs) and diffusion models. These architectures compress data into dense representations, arranging similar points closer together, and then use decoders to sample and create new outputs while preserving key features of the dataset.

The key advantage of autoencoders lies in their ability to process large datasets efficiently, highlight significant features, and reduce storage needs. They can also perform unsupervised training, making them valuable for anomaly detection and classification tasks where labeled data is unavailable. VAEs, in particular, excel at generating new data for applications like image or text synthesis.

However, training deep autoencoder models can be computationally intensive. Additionally, during unsupervised learning, the model might replicate input data without identifying the desired features or miss complex relationships in structured datasets. Despite these challenges, autoencoders remain a powerful tool in the deep learning domain.[11]

Generative Adversarial Networks (GANs)

Generative Adversarial Networks (GANs) are neural networks designed to generate new data that closely resembles the original training data, such as creating realistic images of human faces that do not actually exist. The term “adversarial” refers to the interaction between two components of the GAN: the generator and the discriminator.

The generator produces synthetic data, such as images or audio, often with a creative twist (e.g., transforming a horse image into a zebra). The discriminator, on the other hand, evaluates the generator’s output by comparing it with real data and identifying whether the input is real or fake. This back-and-forth process creates a feedback loop where the generator improves its output while the discriminator becomes better at detecting fakes. Training continues until the generator’s outputs are indistinguishable from real data.

GANs are widely used for generating realistic outputs and enhancing machine learning models. They work effectively with unlabeled or minimally labeled data. However, training GANs can be resource-intensive and may require large datasets. A common issue, known as “mode collapse,” occurs when the generator produces limited and repetitive outputs instead

of diverse ones. Despite these challenges, GANs are a powerful tool in AI for creating high-quality synthetic data.[11]

Success of Deep Learning (DL) in Drug Discovery

AstraZeneca: A global leader in pharmaceuticals, AstraZeneca has successfully integrated AI in drug development, improving everything from virtual screening to clinical trials. Their AI efforts have helped them understand diseases better, identify new drug targets, and accelerate the development process. Their collaboration with AI companies, such as Ali Health, illustrates their ongoing AI adoption for enhanced medical science applications (Nag et al., 2022).

Deargen: A South Korean startup, Deargen developed the MT-DTI model, a DL-based drug-target interaction prediction tool. This model helped identify potential antiviral drugs for COVID-19, including FDA-approved atazanavir and Remdesivir. By predicting interactions using simplified chemical sequences, Deargen's approach has significantly accelerated the drug discovery process (Beck et al., 2020; Scudellari, (2020).

Benevolent AI: A biotechnology company in London, Benevolent AI utilizes AI and machine learning to speed up health-related research. Their AI systems have identified promising drugs for COVID-19, including Ruxolitinib, which is in clinical trials. Their work led to the FDA approval for Baricitinib to be used with Remdesivir, improving recovery rates for COVID-19 patients (Gatti et al., 2021; Richardson et al., 2020).

Skin Cancer Detection: AI-driven smartphone applications are revolutionizing skin cancer diagnosis. Apps like SkinVision use AI algorithms to assess lesions and classify them as high or low risk, offering immediate risk evaluations and medical advice. This advancement enables early detection, which can significantly improve survival rates (Carvalho et al., 2019; Flaten et al., (2020).[10]

Natural Language Processing (NLP)

Natural Language Processing (NLP) is a specialized branch of Artificial Intelligence (AI) that focuses on enabling machines to understand, interpret, and process human languages. This technology involves various tasks, such as analyzing textual information, understanding speech, and interpreting both spoken and written inputs. The primary goal of NLP is to bridge the communication gap between humans and machines.

How NLP Works

NLP systems operate similarly to other AI models, relying on structured, pre-processed data to improve understanding. A key aspect of NLP is Tokenization, where text is divided into smaller, meaningful units called tokens, which aids in interpretation.

NLP models typically operate through two main approaches

Rule-based Systems: This traditional approach uses predefined linguistic rules and algorithms to analyze and generate responses based on language patterns.

Machine Learning Models: These models leverage statistical methods and learn from data, improving over time by incorporating feedback to make more accurate predictions and responses.

NLP is widely used in applications like virtual assistants (e.g., Siri, Alexa), chatbots for customer service, and for analyzing vast amounts of unstructured data, eliminating the need for manual processing.

NLP in Healthcare

In healthcare, NLP enables the processing and analysis of vast amounts of data, including Electronic Health Records (EHRs), clinical notes, imaging records, and other unstructured data. NLP addresses the challenge that approximately 80% of medical data is unstructured, which traditional systems struggle to process effectively.

By extracting meaningful insights from this data, NLP aids in improving decision-making, predicting treatments, and evaluating drug efficacy. It enhances healthcare providers' ability to manage and share information, driving innovations in personalized treatment, improving medication efficacy, and optimizing patient care, ultimately contributing to increased life expectancy and improved quality of life.

Latest NLP Trends in Healthcare

Enhanced Decision-Making: NLP, combined with Big Data and AI, enables healthcare professionals to make faster and more precise decisions, improving treatment and care strategies.

Risk Assessment and Patient Prioritization: NLP, integrated with predictive analytics, helps identify diseases early and prioritize care for high-risk patients, improving healthcare efficiency and patient outcomes.

Improved Clinical Trials: By analyzing unstructured data, NLP enhances the clinical trial process, matching patients with suitable treatments based on their unique conditions, which leads to more successful trials and reduced risks.[12]

Discoveries and Innovations in Medical Practices

NLP accelerates medical discoveries by analyzing large datasets related to drugs, clinical trials, diseases, and treatments. By identifying hidden patterns, NLP reduces the time required for breakthroughs, allowing researchers to focus on implementing findings rather than spending years gathering and analyzing data.

This ability to process unstructured data contributes to faster medical advancements, transforming treatment methods and improving healthcare practices globally.[13]

Key Components of NLP

Tokenization: Dividing text into smaller units (words or phrases) for easier processing.

Sentiment Analysis: Analyzing text to determine its emotional tone (positive, negative, or neutral).

Named Entity Recognition (NER): Identifying and categorizing key elements in text, such as names, locations, and medical terms.

Part-of-Speech Tagging: Assigning grammatical roles (noun, verb, adjective) to words in a sentence to understand sentence structure.

Syntactic and Semantic Analysis: Analyzing sentence structure (syntax) and meaning (semantics) for a deeper understanding of text.

These components form the foundation of how NLP systems process and interpret human language, enabling machines to understand and respond intelligently.[13-14]

SCOPE OF AI IN THE PHARMACEUTICAL INDUSTRY

Artificial Intelligence (AI) is revolutionizing pharmaceutical research by enhancing the efficiency and effectiveness of drug discovery processes. AI technologies, such as machine learning and deep learning, are being integrated into various stages of drug development, from initial target identification to clinical trials.

Scope of AI in Drug Discovery

Drug Discovery and Development: AI accelerates the identification of potential drug candidates by analyzing vast datasets, predicting molecular interactions, and optimizing compound properties. This leads to faster and more cost-effective development cycles.

Drug Repurposing: AI facilitates the identification of existing drugs that can be repurposed for new therapeutic indications, thereby reducing development time and costs.

Clinical Trials: AI enhances the design and execution of clinical trials by predicting patient responses, optimizing dosing regimens, and identifying suitable patient populations, leading to more efficient trials.

Pharmaceutical Productivity: By automating routine tasks and providing predictive analytics, AI improves productivity in pharmaceutical research and development.[15]

Challenges and Limitations of AI in Drug Discovery

While AI holds significant promise in drug discovery, there are several challenges and limitations that must be addressed. One of the primary challenges is the availability and quality of data. AI-driven approaches often require large volumes of data for effective training. However, in many instances, the available data may be limited, incomplete, or inconsistent, which can compromise the accuracy and reliability of the results.

Another major concern is the ethical implications of AI in drug development, particularly regarding fairness and bias. If the data used to train machine learning (ML) algorithms is biased or not representative, the resulting predictions could be skewed or unfair, potentially leading to inaccurate outcomes. It is crucial to ensure that AI is used ethically and fairly when developing new therapeutic agents.

To address these challenges, several strategies can be employed. One solution is data augmentation, which involves generating synthetic data to complement existing datasets. This can enhance the volume and diversity of data available, improving the accuracy of ML predictions. Another approach is the use of Explainable AI (XAI) techniques, which aim to make AI algorithms more transparent by providing interpretable explanations for their predictions. This can help mitigate concerns related to bias and fairness while offering a clearer understanding of how decisions are made by the AI systems.

AI cannot replace traditional experimental methods or the expertise of human researchers. AI can only offer predictions based on the available data, which must still be validated and

interpreted by human scientists. Nevertheless, integrating AI with conventional experimental approaches can improve the drug discovery process, combining the predictive capabilities of AI with the insight and experience of human researchers. This integration has the potential to accelerate the development of new drugs and enhance the overall efficiency of the discovery process.[3]

APPLICATIONS OF AI IN DRUG DISCOVERY

Artificial Intelligence (AI) is revolutionizing the pharmaceutical industry by accelerating and Improving drug discovery and development processes.

Predicting Drug Efficacy: AI algorithms and machine learning models help predict the effectiveness of potential drug candidates, speeding up the drug discovery process.

Improving Clinical Trials: AI can analyze clinical trial data to identify trends, potential adverse effects, and predict drug performance, improving the accuracy and efficiency of these trials.

Tailored Treatments for Specific Patient Populations: AI can analyze large population data to predict which drug candidates are likely to be most effective for specific patient groups, enhancing treatment personalization.

Identifying New Drug Targets: AI plays a key role in discovering new targets for drug development, contributing to the development of innovative treatments.[3]

CONCLUSION

Artificial Intelligence (AI) has revolutionized drug discovery by accelerating processes, reducing costs, and improving precision in identifying and designing drug candidates. Its applications, from target identification to predictive modeling, have streamlined traditional methods, enabling faster and more effective drug development. While challenges like data quality and ethical concerns remain, advancements in explainable AI and data augmentation are addressing these issues. By complementing human expertise, AI is transforming pharmaceutical research, paving the way for innovative therapies and improved global healthcare outcomes.

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