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A Review - Artificial Intelligence in Drug Discovery and Development

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Abstract: *Artificial intelligence (AI) involves the development of smart systems capable of analyzing information, solving complex problems, and supporting decision-making processes. In recent years, AI has gained significant importance in various areas of the pharmaceutical field, including drug discovery, drug development, polypharmacology, and hospital pharmacy. Advanced techniques such as deep neural networks (DNNs) and recurrent neural networks (RNNs) are widely applied to improve research efficiency and accuracy. Several pharmaceutical applications now utilize AI-based technologies in Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) studies to predict the behavior and activity of drug compounds. Furthermore, de novo drug design plays a major role in developing novel drug molecules with optimized and desirable characteristics. This review highlights the applications of artificial intelligence in pharmacy, with special emphasis on drug discovery, formulation development, polypharmacology, and hospital pharmacy services. Artificial intelligence (AI) has become a revolutionary technology in the field of drug discovery and development, offering quicker, more accurate, and economical methods for identifying potential therapeutic compounds. Advanced AI techniques such as machine learning, deep learning, natural language processing, and generative models are widely applied in important stages of drug development, including target recognition, lead compound optimization, virtual screening of chemical databases, and prediction of pharmacokinetic as well as toxicity properties. By processing vast and complex biological data, AI can identify hidden patterns and relationships that are difficult for humans to detect, thereby accelerating the initial stages of drug research and enhancing the precision of scientific decisions.*

Keywords: Drug Development, Rational Drug Design, Machine Learning Techniques, Deep Neural Learning

I. INTRODUCTION

Artificial Intelligence (AI) is defined as the branch of science and technology concerned with developing intelligent machines, particularly advanced computer systems capable of performing tasks that normally require human intelligence. AI also involves using computers to study and simulate intelligent behaviour, without restricting itself only to biologically inspired methods. In 1956, Allen Newell and his team developed the Logic Theorist, recognized as the first artificial intelligence software program. Artificial Intelligence (AI) is defined as the branch of science and technology concerned with developing intelligent machines, particularly advanced computer systems capable of performing tasks that normally require human intelligence. AI also involves using computers to study and simulate intelligent behaviour, without restricting itself only to biologically inspired methods. In 1956, Allen Newell and his team developed the Logic Theorist, recognized as the first artificial intelligence software program.

The drug discovery process is highly extensive and usually takes around 12 years to complete. It starts with preclinical studies such as hit identification, lead discovery, and lead optimization, followed by Phase I, Phase II, and Phase III clinical trials before a drug is finally approved for human use. This entire procedure is very costly, with expenses reaching nearly 1.2 billion dollars, and many drugs are later withdrawn due to harmful side effects in humans.

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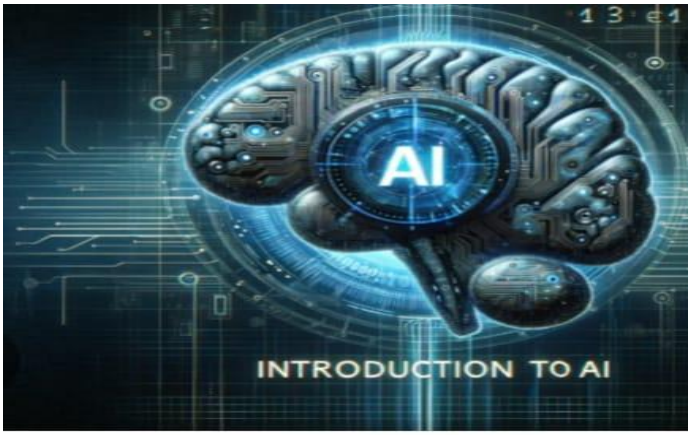
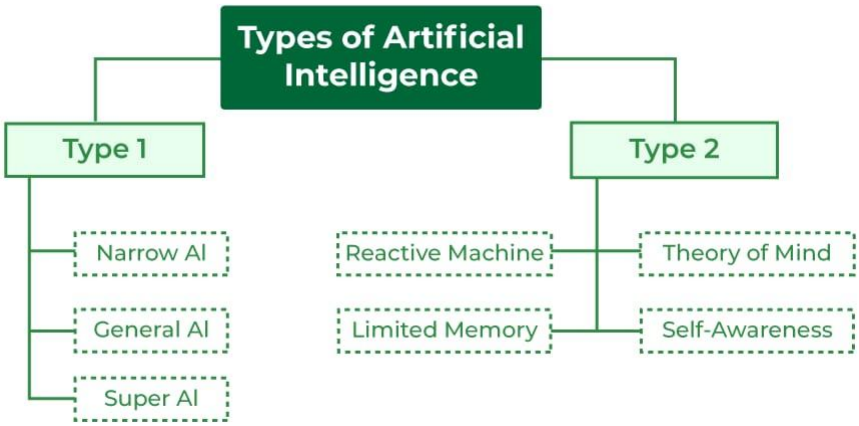
Therefore, advanced technologies like Artificial Intelligence (AI), including Machine Learning (ML) and Deep Learning (DL), have become valuable tools for accelerating drug development while also reducing overall costs. Artificial Intelligence (AI) is expected to revolutionize the field of drug discovery. One of the major challenges in developing a new medicine is the large amount of time and money required to evaluate its safety and effectiveness in patients before approval. The pharmaceutical industry is rapidly adopting artificial intelligence (AI) at an unprecedented pace. AI systems are capable of generating fast predictions, although these predictions may sometimes lack accuracy. However, AI-generated predictions can be validated through clinical trials before being applied to patients, as long as they remain within the boundaries of the research and development process.



Classification: Artificial Intelligence (AI) can be classified in several ways



❖ **Evolution of AI**

You may be surprised to know that the idea of Artificial Intelligence (AI) is very old. Ancient Greek and Egyptian myths even described mechanical humans and intelligent machines. The following milestones explain the development of AI from its early beginnings to the modern era.

❖ **AI Maturation (1943–1952)**

- In 1943, Warren McCulloch and Walter Pitts introduced the first mathematical model of an artificial neuron, which became the foundation of modern AI.

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- In 1949, Donald Hebb proposed a method for adjusting the strength of connections between neurons. This learning principle later became known as Hebbian learning.

❖ **Early Enthusiasm and the Golden Years (1956–1974)**

- In 1966, researchers concentrated on developing algorithms capable of solving mathematical problems.
- In the same year, Joseph Weizenbaum created the first chatbot, called ELIZA.
- In 1972, the first intelligent humanoid robot, WABOT-1, was developed in Japan.
- The First AI Winter (1974–1980)

❖ **Development of Artificial Intelligence (1980–1987)**

- In 1980, AI regained popularity with the emergence of Expert Systems after a period of decline.
- Expert systems were created to imitate the decision-making abilities of human experts.
- In 1980, Stanford University hosted the first national conference of the American Association for Artificial Intelligence.

❖ **Second AI Winter (1987–1993)**

- The second AI winter lasted from 1987 to 1993.
- Expert systems such as XCON eventually became too expensive and less practical.
- In 1997, IBM's Deep Blue defeated world chess champion Garry Kasparov, becoming the first computer to beat a reigning world champion in chess.

❖ **Advantage of AI tecgnology:**

1. Minimize Errors
2. Hard Exploration
3. Daily Applications
4. Digital Assistants
5. Repeated Tasks and Multitasking
6. Medical Uses
7. Continuous Working Ability
8. Increase Technological Growth
9. Working in Dangerous Areas
10. Educational Support

❖ **Disadvantages of AI technology:**

1. High cost
2. Lack of human emotions
3. Unemployment risk
4. Dependence on machines
5. No creativity
6. Privacy and security issues
7. Bias and errors
8. Continuous maintenance required
9. Limited decision-making ability
10. Environmental impact

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❖ **AI in drug discovery :**

The vast chemical space contains more than 1060 molecules, which provides opportunities to design many potential drug compounds. However, drug development is restricted by the lack of advanced technologies, making it expensive and time-consuming—areas where AI can provide support. AI helps in identifying hit and lead compounds, faster validation of drug targets, and optimization of drug structure design. Various applications of AI in drug discovery are shown. Despite its advantages, AI faces challenges due to the size, complexity, growth, and unpredictability of data. Pharmaceutical companies often manage datasets containing millions of molecules, which can be difficult for traditional machine learning methods to process. Computational models such as quantitative structure-activity relationship (QSAR) can quickly predict a large number of compounds or basic physicochemical properties like log P and log D. A computer model based on Quantitative Structure–Activity Relationship (QSAR) can rapidly predict large numbers of chemical compounds and simple physicochemical properties such as log P and log D. However, these models are limited in their ability to predict complex biological properties like chemical activity and side effects. In addition, QSAR models often suffer from small training datasets, errors in experimental data, and insufficient experimental validation.

To overcome these limitations, emerging artificial intelligence techniques such as deep learning (DL) and related modeling approaches are being used to improve the safety and effectiveness of drug compounds through big data analysis. For example, Merck organized the QSAR ML 2012 competition to explore the advantages of machine learning and deep learning in pharmaceutical development. In Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) datasets containing 15 drug candidates, deep learning models showed better predictive performance compared to traditional machine learning methods.

The concept of chemical space describes the distribution of molecules and their properties, similar to a geographical map of compounds. Chemical space visualization helps in understanding molecular information and identifying bioactive compounds. Virtual screening (VS) uses this concept to select promising molecules for further testing.
Several public chemical databases such as PubChem, ChemBank, DrugBank, and ChemDB provide access to large collections of compounds. Various in silico methods, including structure-based and ligand-based approaches, are used in virtual screening to improve compound profiling and quickly eliminate unsuitable lead compounds, reducing cost and time in drug discovery.

Drug design techniques like molecular fingerprints and Coulomb arrays are used to select lead compounds and analyze their physicochemical and toxicological properties. Multiple computational features, including molecular similarity and predictive modeling, are applied to estimate the chemical structure and biological activity of substances using in silico methods.

❖ **Role of drug discovery:**

- Target identification
- Drug molecule design
- Virtual screening of compounds
- Drug repurposing
- Prediction of drug activity
- Toxicity and side-effect prediction
- Pharmacokinetic prediction (ADME)
- Lead optimization
- Biomarker discovery

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❖ **AI in Drug Discovery Stages:**

A. Target Identification:-

This helps researchers detect disease-related targets much earlier and more efficiently than traditional methods.

Examples include:

Genomic data

Proteomic information

Biological pathway datasets

Biomarker identification

B. Virtual Screening

AI rapidly evaluates millions of chemical compounds to discover potential drug candidates using:

Deep learning

Reinforcement learning

Graph neural network techniques

C. Drug Repurposing:-

AI identifies alternative therapeutic uses for already approved medicines, helping reduce both development time and overall cost.

Examples include:

COVID-19 drug repurposing studies

Cancer treatment research

Antiviral drug discovery projects

❖ **Tools used in AI Driven drug delivery :**

Tools	Application
Deep Learning	Identifies features and predicts drug–target interactions
AlphaFold	Predicts 3D protein structures
Generative Models (GANs, RNNs)	Designs new drug molecules
Graph Neural Networks	Performs structure-based molecular analysis

❖ **Artificial Intelligence in Clinical Trial Design –**

- **Defination:**

A clinical trial is a systematic research study conducted on human volunteers to evaluate the safety, efficacy, dosage, and side effects of a new drug, vaccine, medical device, or treatment before it is approved for public use

- **Phases of clinical trial:**

Phase	Main purpose	Participants
Phase 0	Preliminary exploratory study	10–15 volunteers
Phase I	Safety and dosage	20–100 healthy volunteers
Phase II	Efficacy and side effects	100–300 patients
Phase III	Confirmation of efficacy and safety	1,000–3,000 patients
Phase IV	Post-marketing monitoring	General population

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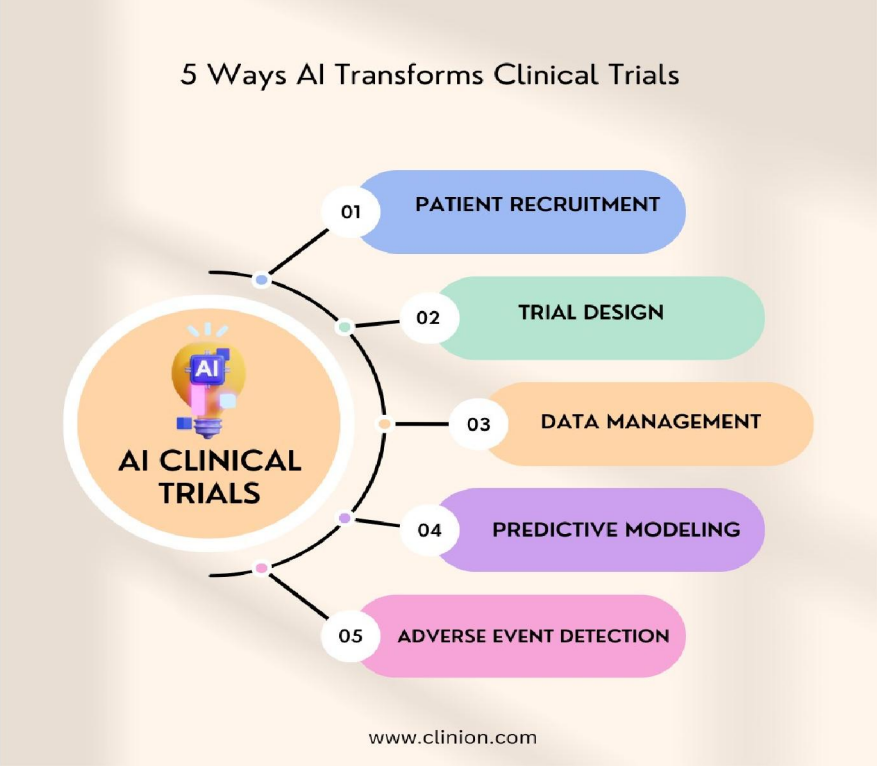
❖ **Artificial Intelligence in Clinical Trial Design –**

Clinical trials usually require 6–7 years and huge financial resources to evaluate whether a medicine is safe and effective for treating a disease. Despite this major investment, only a small number of tested molecules successfully reach approval, causing considerable losses for pharmaceutical companies. Many clinical trial failures occur because of inappropriate patient selection, inadequate infrastructure, or technical limitations. The growing availability of digital healthcare data has created opportunities for Artificial Intelligence (AI) to minimize these problems and improve trial outcomes.

Patient recruitment is one of the most time-consuming stages of clinical trials, occupying nearly one-third of the total study duration. Selecting suitable participants is essential because poor recruitment is responsible for a large percentage of unsuccessful trials. AI technologies can analyze genomic information, medical histories, and patient exposure profiles to identify individuals who are more likely to respond positively to a treatment. This approach is especially valuable in Phase II and Phase III clinical trials, where accurate patient selection increases the probability of success.

AI-based predictive machine learning models also support preclinical research by identifying promising lead compounds before they enter human testing. These systems help researchers predict therapeutic potential and choose the most suitable candidates for specific patient populations. In addition, participant dropout during clinical studies contributes significantly to trial failure, increasing both costs and delays. AI-powered monitoring tools can improve patient compliance with treatment protocols through continuous tracking and reminders. For example, the mobile platform developed by AiCure was used in a Phase II schizophrenia trial and significantly improved medication adherence, helping ensure smoother completion of the study.



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❖ **Impact of AI on Drug Discovery & Development:**

A. AI in Drug Discovery

Traditional drug discovery methods have historically been slow, expensive, and labor-intensive. Developing a new drug from initial research to market approval often takes many years or even decades. The process involves several stages such as target identification, validation, lead compound discovery, efficacy testing, and clinical trials. A large number of drug candidates fail during these stages, particularly in clinical trials, mainly because of safety concerns or lack of effectiveness.

Conventional approaches also faced limitations in handling large and complex biological data, as they relied heavily on linear models and experimental observations. This restricted the ability to accurately predict drug interactions, side effects, and therapeutic potency.

B. FUNCTIONS OF AI IN DRUG DISCOVERY:

Artificial intelligence has shown great potential in speeding up the drug discovery process while improving the accuracy and efficiency of different stages of drug development. However, further research is still required to address ethical and legal concerns and to improve AI models for the discovery of new medicines. AI research in drug development mainly focuses on creating transparent and explainable models so that researchers can clearly understand how predictions and decisions are made.

Functions:

Data Analysis: AI can process and analyze large volumes of biological and clinical data quickly and accurately.

Evidence-Based Decision Making: AI helps researchers make informed decisions using reliable scientific data and predictive models.

Better Clinical Trial Design: AI improves patient selection, trial monitoring, and prediction of treatment outcomes, making clinical trials more efficient.

C. INTERPRETABILITY ISSUE:

Interpretability is one of the key characteristics of AI models used in drug discovery. It allows researchers to understand how AI systems generate predictions and decisions. Better interpretability increases the reliability and trustworthiness of AI models and also provides valuable insights into the biological mechanisms involved in drug action.

D. Drug Design and Optimization

Machine learning models predict the properties, effectiveness, and toxicity of compounds, helping scientists design safer drugs.

E. Prediction of Drug Interactions

AI can predict how drugs interact with the human body and with other medicines.

F. Improved Clinical Trials

AI assists in patient selection, monitoring, and analysis of clinical trial data, increasing success rates.

G. Automation of Research

AI-powered robots and systems automate laboratory experiments and data collection.

AI provides data-driven insights that help researchers make accurate scientific decisions.

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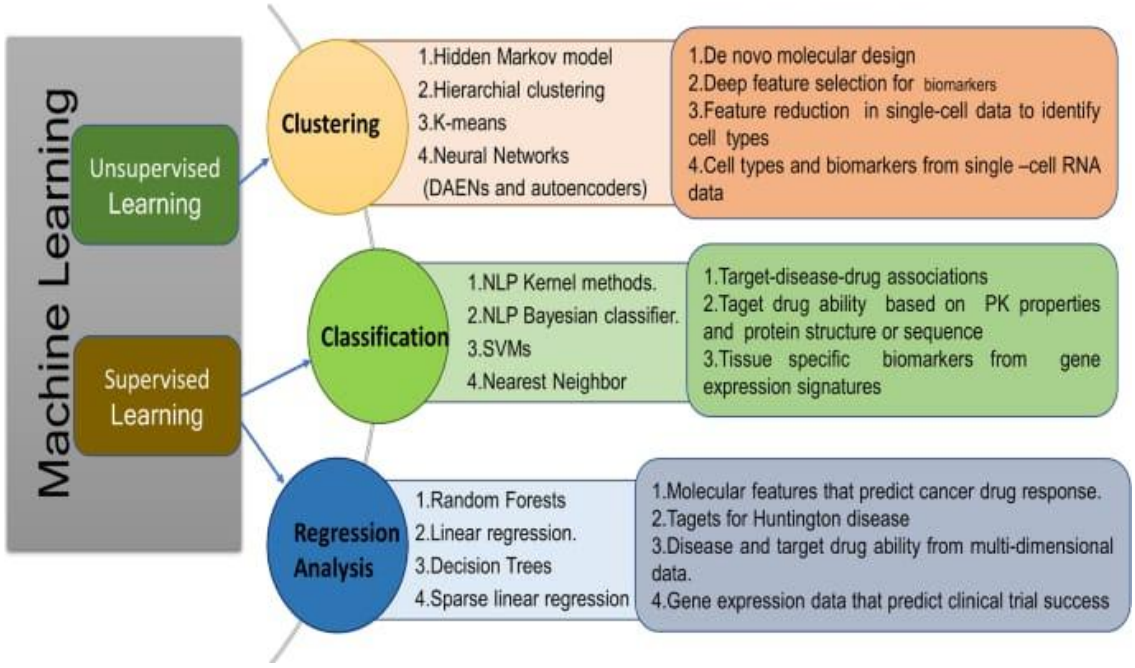
❖ **Machine Learning and Deep Learning Applications of Artificial Intelligence:**

Artificial Intelligence (AI) is the process of enabling machines to perform tasks that normally require human intelligence. The main goal of AI is to create systems that can think, learn, and solve problems similarly to humans. These intelligent systems can analyze information, make decisions, and perform tasks automatically.

Machine Learning (ML) is a subset of AI in which machines learn from data without being explicitly programmed. ML algorithms analyze large amounts of data, identify patterns, and use those patterns to make predictions or decisions.

Deep Learning (DL) is an advanced form of machine learning that uses artificial neural networks inspired by the human brain. Deep learning models generally provide higher accuracy than traditional machine learning models, especially when large datasets are available. However, they require greater computational power and more training data. While machine learning performance may eventually reach a limit, deep learning models continue to improve as the amount of data increases.



Challenges of AI in Drug Discovery:

Although Artificial Intelligence (AI) offers many advantages in drug discovery, several challenges and limitations still exist. AI-based systems require a large amount of high-quality data for proper training. However, available medical and pharmaceutical data are often limited, incomplete, or inaccurate, which can reduce the reliability and accuracy of predictions.

Another major concern is ethics and fairness. If machine learning models are trained using biased or non-representative data, the predictions generated may become unfair or misleading. Therefore, ensuring ethical and unbiased use of AI in drug development is extremely important.

One approach to overcome data-related problems is data augmentation, where artificial or synthetic data are generated to increase the quantity and diversity of training datasets. This helps improve the performance and dependability of AI models.

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Another useful strategy is Explainable AI (XAI), which provides clear and understandable explanations for AI predictions. Explainable AI helps researchers understand how decisions are made by machine learning systems and reduces concerns regarding bias and transparency.

Despite its capabilities, AI cannot completely replace traditional laboratory experiments or the expertise of scientists and researchers. AI systems mainly make predictions based on existing data, while human experts are required to verify, interpret, and apply the findings correctly.

Therefore, combining AI technologies with conventional experimental methods can improve the overall drug development process. The integration of AI's predictive power with human knowledge and scientific experience can accelerate the discovery of new medicines and make drug development more efficient.

Collaboration Between AI Companies and the Pharmaceutical Industry:

Collaboration between Artificial Intelligence (AI) companies and pharmaceutical industries has become increasingly important in modern drug discovery and development. AI companies provide advanced technologies such as machine learning, deep learning, and data analytics, while pharmaceutical companies contribute medical knowledge, clinical experience, and large healthcare datasets.

These partnerships help accelerate the drug discovery process by identifying potential drug candidates more quickly and accurately. AI tools can analyze massive biological and chemical datasets, reducing the time and cost required for research and development.

Collaboration also improves target identification, drug design, clinical trial management, and prediction of drug safety and effectiveness. Pharmaceutical companies benefit from AI-driven insights, whereas AI companies gain access to valuable scientific and clinical data for improving their models.

In addition, such partnerships support personalized medicine by developing treatments tailored to individual patients based on genetic and medical information. Many pharmaceutical organizations now work with AI startups and technology firms to develop innovative therapies for complex diseases.

However, successful collaboration requires proper data sharing, transparency, ethical practices, and regulatory compliance. Combining the technological expertise of AI companies with the scientific knowledge of pharmaceutical industries can significantly improve the efficiency and success of drug development.

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❖ **Applications of Drug Discovery and Development:**

1. **Treatment of Diseases**

Drug discovery helps in developing medicines to treat infectious, chronic, genetic, and life-threatening diseases.

2. **Prevention of Diseases**

Development of vaccines and preventive medicines reduces the spread of diseases and improves public health.

3. **Personalized Medicine**

Modern drug development uses genetic and patient-specific data to create targeted therapies for individuals.

4. **Cancer Therapy**

Discovery of anticancer drugs helps in targeted treatment with fewer side effects and better survival rates.

5. **Management of Chronic Disorders**

Drugs are developed for long-term conditions such as diabetes, hypertension, asthma, and arthritis.

6. **Improvement in Quality of Life**

Medicines reduce symptoms, relieve pain, and improve the overall health and comfort of patients.

7. **Control of Infectious Diseases**

Antibiotics, antivirals, and antifungal drugs help in controlling bacterial, viral, and fungal infections.

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8. Drug Repurposing

Existing drugs are studied for new therapeutic uses, reducing development time and cost.

9. Advancement in Biotechnology

Drug development supports innovations such as monoclonal antibodies, gene therapy, and biologics.

10. Economic and Healthcare Benefits

Successful drug development reduces healthcare burden, creates employment, and supports pharmaceutical industries.

II. CONCLUSION

Artificial intelligence in drug discovery is not a new concept. For many years, machine learning has played an important role in identifying and designing small-molecule targets. With recent advancements, AI has become more powerful and efficient, helping reduce costs and improve productivity across different stages of drug development. In addition to molecule identification and toxicity prediction, biotechnology companies are now exploring several innovative AI-based applications in drug research. This transformation is also changing the strategies of large pharmaceutical companies, which increasingly obtain trial-ready compounds from external sources instead of performing all research internally. AI techniques have tremendous potential to accomplish these objectives, but their effectiveness relies on matching the appropriate technology with the correct scientific problem. In recent years, the application of artificial intelligence in important pharmaceutical fields such as drug discovery, formulation development, polypharmacology, and hospital pharmacy has gained significant attention. AI-based approaches attempt to imitate human intelligence by enabling machines to process information, solve complex problems, and make logical decisions. Consequently, the use of AI has simplified the development of new hypotheses, strategic planning, prediction models, and the evaluation of multiple related factors while reducing both time and overall cost.

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