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IMPACT OF ARTIFICIAL INTELLEGENCE (AI) AND MACHINE LEARNING (ML) IN PHARMACEUTICAL SCIENCES

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Abstract

Artificial Intelligence (AI) involves machines, especially computer systems, simulating human intelligence processes like expert systems, natural language processing, speech recognition, and machine vision. Its history traces back to the 1950s, emphasizing symbolic approaches and problem-solving. The US Department of Defence engaged in AI research in the 1960s, focusing on teaching computers human reasoning. Projects like DARPA's street mapping in the 1970s paved the way for intelligent personal assistants in 2003.
AI operates by analysing vast datasets to detect patterns and correlations, utilizing specialized hardware and software with languages such as Python, R, Java, C++, and Julia. AI systems can predict future events or behaviours, like chatbots learning from text examples or image recognition tools identifying objects. Cognitive skills such as learning, reasoning, self-correction, and creativity are vital in AI programming.
John McCarthy coined the term "Artificial Intelligence" in the mid-1950s, defining it as creating intelligent machines. AI applications span industries like healthcare and automobiles. In healthcare, AI aids patient monitoring and surgical assistance, while in automobiles, it enables Advanced Driving Aid Systems (ADAS) and autonomous driving.
In marketing, AI leverages data analysis and predictive modeling to personalize strategies and enhance customer experiences. AI technologies are continuously evolving, offering specialized benefits across sectors and transforming industries with their innovative capabilities.

Keywords: Artificial Intelligence, Machine Learning, Expert System, Natural Language Processing, Cognitive Skills, Healthcare Applications, Automotive Applications.

Introduction to AI

What is artificial intelligence (AI)?

The simulation of human intelligence processes by machines, particularly computer systems, is known as artificial intelligence. Expert systems, natural language processing, speech recognition, and machine vision are a few specific uses of AI[1].

Artificial Intelligence History

1. In the 1950s, symbolic approaches and problem solving were the focus of early AI research. The US Department of Defence became interested in this kind of work in the 1960s and started teaching computers to simulate fundamental human reasoning. For instance, in the 1970s, the Defence Advanced Research Projects Agency (DARPA) finished street mapping projects. In 2003, DARPA developed intelligent personal assistants, far before Siri, Alexa, or Cortana were well-known.

2. The automation and formal reasoning that we see in computers today, such as intelligent search and decision support systems that may be built to supplement and even enhance human talents, were made possible by this early work.

Although AI is portrayed in science fiction books and Hollywood films as human-like robots that take over the world, AI technologies aren't all that smart or frightening at this point in their development. Rather, AI has developed to offer numerous specialized advantages across all sectors. For instances of artificial intelligence in retail, healthcare, and other fields today, continue reading.[2]

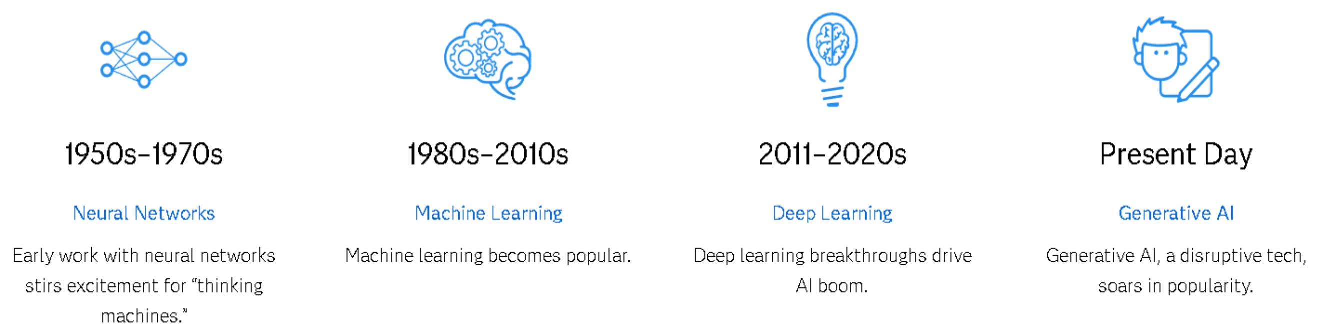


Figure: Early work with neural networks, Machine learning gains popularity, Breakthroughs propel the AI explosion, Generative AI is becoming increasingly popular[2]

How the AI work?

- AI works by analysing large amounts of labelled training data to find patterns and correlations.
- It requires specialized hardware and software, with popular programming languages like Python, R, Java, C++, and Julia often used by developers.
- AI systems can use this data analysis to make predictions about future events or behaviour. For example, a chatbot learns to have lifelike conversations by studying text examples, and an image recognition tool identifies objects in images by reviewing numerous examples.[3]
- AI programming focuses on cognitive skills like learning, reasoning, self-correction, and creativity to achieve specific tasks, such as generating new text, images, music, and ideas.

Where did the term "Artificial Intelligence" come from?

John McCarthy, widely recognized as the father of Artificial Intelligence due to his astounding contribution in the field of Computer Science and AI. [4]It was in the mid-1950s that McCarthy coined the term "Artificial Intelligence" which he would define as "the science and engineering of making intelligent machines".

Application of AI

1. AI in Healthcare

Patient Monitoring: In case of any abnormal activity and alarming alerts during the care of patients, an AI system is being used for early intervention. Besides this, RPM, or Remote Patient Monitoring has been significantly growing & is expected to go up by USD 6 Billion by 2025, to treat and monitor patients.

Surgical Assistance: Surgeons can make informed decisions based on the insights supplied by the AI algorithms, ensuring a streamlined operation and avoiding additional risks during processing
.

2. AI in pharma practice

The use of AI technology gives pharmacists tools and systems that assist them make accurate and evidence-based healthcare judgments. Using AI algorithms and machine learning, pharmacists can swiftly examine vast volumes of patient data, such as medical records, test findings, and drug profiles. This enables them to detect possible drug-drug interactions, evaluate the safety and efficacy of medications, and make educated recommendations to specific patients.

3. AI in Automobiles

ADAS system: The Advanced Driving Aid System, also known as ADAS, is an artificial intelligence programmed that is well-known for handling sensitive and important data, such as crash detection, parking aid, and driving assistance. Because of the way the algorithm is built, it will begin alarming automatically in order to stop any collisions.

Autonomous Driving: By using AI, it is possible to navigate and drive cars automatically without the need for actual human intervention. LIDAR, RADAR, and other sensors, among others, assist in gathering more information to assess the environment and make the best decisions in the real world.[5]

4. AI in marketing

With AI's ability to gather and monitor tactical data in real-time, marketers can make decisions now, instead of waiting until the campaign is finished. Data-driven reports may be used to inform their decisions on what to do next, helping them make better, more unbiased choices.

One example of using AI in marketing is Smart Compose in Gmail and Google Docs, which uses machine learning to read what you type, understand it, and recommend what to put next.[6]

5. AI in education

Grading can be automated by AI, giving the tutor more time to instruct. As a teaching assistant, an AI chatbot can converse with students.

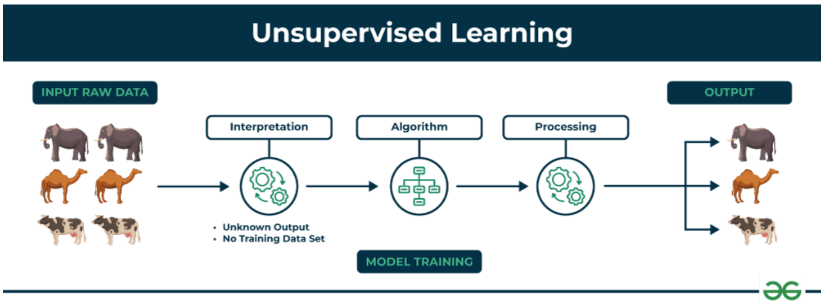
In the future, artificial intelligence (AI) may serve as a convenient, anytime, anywhere personal virtual tutor for pupils.

6. AI in agriculture

For the best results, agriculture is an industry that needs a variety of resources, including labor, money, and time. Agriculture is going digitized these days, and artificial intelligence is developing in this space. AI is being applied to agriculture through predictive analysis, solid and crop monitoring, and argon robotics. For farmers, AI in agriculture can be highly beneficial.

7. AI in business management

AI is giving the e-commerce sector a competitive edge, and it is becoming more necessary for e-commerce enterprises. AI is assisting consumers in finding related products with suggested brand, color, and/or size[7].



Machine learning

A subfield of computer science and artificial intelligence (AI) called "machine learning" focuses on using data and algorithms to simulate human learning processes and progressively increase their accuracy[8].

The most widely used form of AI technology in use today is probably machine learning. You may have come across a few of the most prevalent instances of machine learning in your daily life, such as:

- Recommendation engines that suggest products, songs, or television shows to you, such as those found on Amazon, Spotify, or Netflix

- Speech recognition software that allows you to convert voice memos into text.

- A bank's fraud detection services automatically flag suspicious transactions.

- Self-driving cars and driver assistance features, such as blind-spot detection and automatic stopping, improve overall vehicle safety[9].

Types of machine learning

- Supervised learning:

As the name implies, supervised learning is far more like to a machine under human supervision. More accurately, people direct the algorithm by suggesting conclusions for it to draw. Algorithms with preset outputs and data labelled with correct responses are necessary for supervised learning. Task regression is the term we can use if the output result is a number. Classification is used when there is only one or a small number of unordered items in the output[10].

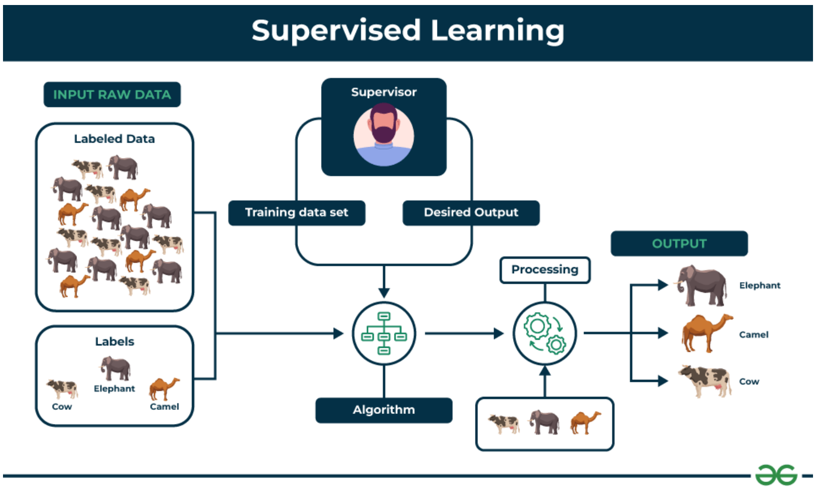


Figure: Supervised learning[11]

- Unsupervised learning:
  Unsupervised learning is more closely associated with the concept of "true artificial intelligence," which is the belief that a computer is capable of recognizing intricate patterns and processes without the need for human supervision or help. About the artefacts, not much information is available. Specifically, the train set is label less. It is possible to identify and arrange items into appropriate clusters based on their commonalities across data groups. Anomalies are those items that differ noticeably from every cluster.

Reinforcement learning:

Reinforcement learning uses goal-oriented algorithms that are trained over an extended period of time to learn how to maximize along a certain dimension or accomplish a complex aim. This kind of machine learning does not need training datasets, in contrast to supervised learning. Supervised learning, on the other hand, uses a different approach and focuses on teaching the software the right answer. Reinforcement training does not provide such a solution. Without the use of training data, the reinforcement agent makes decisions about what to do in the provided data based only on its own experience[12].

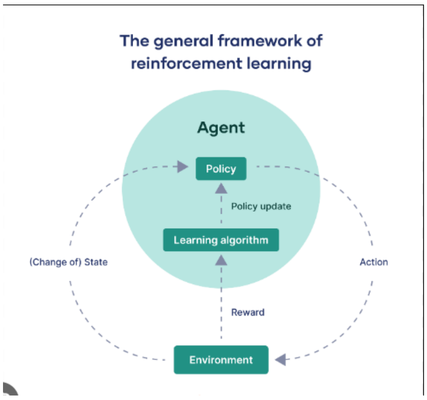


Figure: The General framework of reinforcement learning[13]

Application of Ml:

1. Genetics and Genomics: To determine the underlying effects of heredity on human health, machine learning in genomics influences a number of fields, including genome sequencing, genetic research, and gene manipulation. Predictive testing for early disease diagnosis is another newly developed application that aims to enhance the standard of patient care.
2. Cancer Prognosis and Prediction: ML algorithms are used in cancer research because they can find important characteristics in complex datasets. Using methods like Artificial Neural Networks (ANNs), Bayesian Networks (BNs), and Decision Trees (DTs), it is utilized to build prediction models. This aids in accurate decision-making and modelling of the development and treatment of cancerous illnesses[12].
3. Drug discovery/manufacturing: Millions of compounds must undergo an expensive and time-consuming sequence of testing in order to produce or find a new medication. ML can expedite this complex, multi-step drug discovery process.

How are AI and ML connected?

Although AI and ML are not exactly the same, they share many similarities. The easiest method to comprehend the relationship between AI and ML is as follows[14]:

- Enabling a machine or system to think, feel, behave, or adapt like a human is known as artificial intelligence (AI).

- Machine learning (ML) is an AI application that enables computers to automatically extract knowledge from data and learn from it.

Thinking of machine learning and artificial intelligence as broad concepts might help you remember their distinctions. The general term "artificial intelligence" refers to a broad range of particular techniques and algorithms. Under that general heading, machine learning is included, along with other prominent subfields including deep learning, robotics, expert systems, and natural language.

How can organizations use AI and ML?

- To better target your sales and marketing efforts, segment your customer base based on their traits, behaviours, and preferences. This process is known as customer segmentation.
- Fraud detection is the process of identifying, classifying, and resolving anomalous transactions.
- Sentiment analysis is the process by which user feedback is integrated into marketing and product strategy.
- Chatbots are useful for triaging and customer support queries[15].

Some drawback of AI and ME in industry

1. No Ethics: Morality and ethics are significant aspects of human nature that are challenging to replicate in artificial intelligence. Many people fear that as AI develops quickly, it will someday become uncontrollable and exterminate humanity[16].
2. Make Humans Lazy: Most laborious and repetitive operations are automated by AI software. We tend to engage our brains less and less because we do not need to memories information or solve puzzles to complete tasks. Future generations may experience issues as a result of this AI addiction.
3. High cost: AI is very expensive since it requires the newest hardware and software to function and stay current with requirements.

Unleashing innovation - AI and ML in pharma sciences

Revolutionizing drug discovery:

The integration of artificial intelligence (AI) and machine learning (ML) is reshaping the landscape of drug development, marking a pivotal moment in medical innovation. These powerful tools are revolutionizing traditional paradigms by accelerating research and enhancing efficiency. With the potential to personalize medicine, AI and ML are driving a new era of drug discovery, promising transformative advancements at the intersection of technology and healthcare[17].

- FDA and EMA Recognition: The FDA in the United States and the EMA in the European Medicine Agency recognise the growing use of AI and ML in drug development. The incorporation of these technologies into regulatory filings has increased noticeably.
- Wide Range of Applications: AI and ML are being used in medication development at several phases, from early discovery to post-market surveillance. These technologies encompass a broad range of tasks, such as manufacturing, safety monitoring, and clinical research.
- Use in Data Analysis and Interpretation: Throughout the lifetime of pharmaceutical goods, AI/ML systems support data collecting, transformation, analysis, and interpretation. They are especially helpful in modelling strategies that lessen or improve the preclinical development's use of animal models[18].
- therapeutic Discovery and Target Identification: By examining genetic, genomic, and proteomic data, AI/ML systems assist in the identification of possible therapeutic targets. By predicting target efficacy and optimising lead compounds, they facilitate the early stages of drug development for researchers.
- Clinical study Optimisation: By evaluating patient data, these tools enhance patient recruitment, forecast patient reactions, and enhance study designs. They improve productivity, cut expenses, and raise clinical trial success rates.
- Risks and Challenges: Although integrating AI/ML into drug development has many advantages, there are risks associated with it as well, including data bias, interpretability issues, regulatory concerns, and technical difficulties. To guarantee the safe and efficient application of AI/ML in pharmaceutical innovation, these issues must be properly addressed.
- Possibility for Personalised Medicine: By facilitating efforts in personalised medicine, AI/ML has the potential to completely transform the drug development process. These technologies open the door to more individualised and effective treatments by anticipating molecular interactions and analysing complex biological data[19].

Target identification in drug discovery

- Target identification is the process of finding molecules—usually proteins—that, if their activity were altered, could change a disease state. To find possible targets that are probably involved in disease processes, machine learning algorithms can analyses a variety of data sets, such as gene expression profiles, protein-protein interaction networks, and genomic and proteomic data [20]. Just about 3,000 of the 20,000 or so proteins that make up the human proteome have been found to be viable targets for treatment[21]. Our understanding of which proteins might be used as therapeutic targets may be expanded by new discoveries.

- Establishing a causal link between the target and the illness is the first stage in defining a target [22]. Graphs, GNNs, or tree-based techniques can be used to determine the causal links between genes and diseases. To anticipate morbidity-associated genes that are also druggable, a decision tree-based meta-classifier was developed in[23]. It was trained on a network topology comprising protein-protein, metabolic, and transcriptions connections, as well as tissue expression and sub-cellular localization of proteins. Key features from the decision tree were found to be extracellular location, centrality in metabolic pathways, and regulation by numerous transcription factors (TFs). Proteins for particular diseases, like lung, pancreatic, and ovarian cancer, were categorized as therapeutic targets or non-targets by machine learning-based techniques based on characteristics like protein-protein interaction, gene expression, DNA copy number[24].

- The literature is the main source of data regarding target association with disease. To find pertinent target-disease pairings in the literature and create databases for target identification, text mining and Natural Language Processing (NLP) techniques can also be applied [25]. Drug-disease, gene-disease, and target-drug connections can be found in papers by mining them with Be Free[26].PKDE4J and other deep learning-based methods[27].
- Without specifically addressing the target identification of those reference ligands, drug-target interactions can also be inferred inside the same cell based on descriptor similarity to those ligands. Using a method inspired by neural networks, a software tool (Spider) [28,] discretizes the input feature similarity vector onto a so-called feature map.

AI and machine learning in pharmaceutical sciences are revolutionizing drug discovery:

- Target Identification: Identifying new targets faster and more precisely.
- Lead optimization: The process of efficiently sifting through enormous chemical spaces.
- Drug repurposing: It is the discovering new applications for existing drugs.
- Patient stratification: The process of identifying individuals who are most likely to react to therapy.
- Predicting Clinical Outcomes: Creating More Effective and Informative Trials.
- Real-time monitoring: It allows for the early detection of probable harmful occurrences.
- Personalized medicine: Entails tailoring therapy based on specific patient data.

Personalized medicine:

The ideal environment for personalized medicine and health care is one in which individual patients' diagnoses, treatment, and follow-up monitoring are simplified into a single process with highly seamless and coordinated transitions from one important activity or sub-process to the next. A promising paradigm for this is the development of cell replacement treatments for a wide range of illnesses. For example, in certain immunotherapeutic-oriented cell replacement treatments for cancer, a patient's tumor is profiled for the presence of distinct 'neo-antigens' or mutations that may entice the host's own immune system to attack cells containing such alterations. If such neoantigens are discovered, cells from either a donor (allogeneic transplantation) or the patient themselves (autologous transplantation) are extracted and sensitized to detect the neoantigens. When put into the patient's body, these cells attract immune cells to tumor cells containing neo-antigens [29,30].

Drug safety: Drug safety is a significant barrier in bringing novel medications to market. Unexpected toxicities are a major cause of attrition during clinical trials, and post-marketing safety concerns result in avoidable morbidity and mortality.
There are two complementary strategies for addressing medication safety (Figure 3). Before a medicine is licensed, clinical trials demonstrate that it is both safe and effective for its intended purpose. Once a medicine is released, it is monitored through AE reports to verify that the safety information is current, a procedure known as pharmacovigilance (PV).
Trials have concentrated on creating medications for the typical patient [31], despite growing requests for precision medicine to enable the "right drug at the right dose to the right patient" [32]. Once pharmaceuticals have been authorized, it is up to programs to monitor their safety. These organizations use databases of spontaneously gathered AE complaints to identify leads and do confirmatory follow-up investigations. However, spontaneous accounts might be biased, leading to underreporting of infrequent occurrences and drug-drug interactions (DDIs) [33].

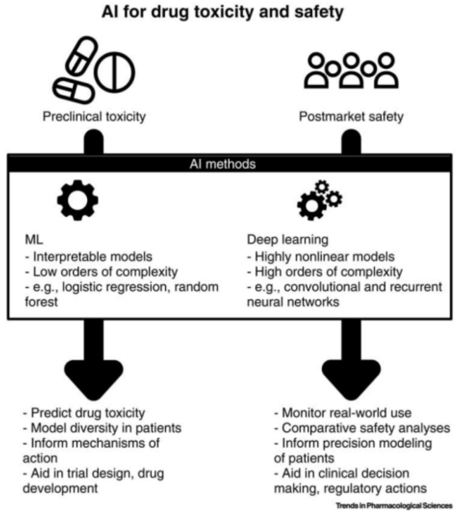


Figure: AI for drug toxicity and safety[34]

Pre-clinical drug safety:

AI approaches have been demonstrated to play a crucial role in pre-market medication safety, particularly in toxicity evaluation. medication toxicity determination is a critical phase in medication design and entails determining the adverse effects of compounds on humans, plants, animals, and the environment[35]. Pre-clinical studies are essential for preventing harmful medications from entering clinical trials. Despite this, severe toxicity remains a key cause of medication failure, accounting for two-thirds of post-market withdrawals, and one-fifth of clinical trial failures[36].Thus, precise toxicity estimations are critical for maintaining medication safety and can assist minimize the cost and development time required to bring new treatments to market. Animal studies have long been the most common way to measure toxicity[37].

Artificial Intelligence: Regulatory Landscape

The advancement of AI technology necessitated the creation of the first legal acts in this field. Each country has its own approach to this issue, considering its legal system. By 2020, the world will have had extensive expertise in regulating new connections related to AI. The experience includes national AI policies and guidelines for implementing AI in various fields. The next section will provide a quick overview of legal texts related to AI.

National Strategic Development Documents:

These papers play a significant role in regulating AI technology through legislation. Approximately two dozen nations now have national development strategies. These nations include China, Korea, Canada, the US, the UK, France, and, as of 2019, Russia.

- Strategic development documents often include strategies for developing AI technology. They may include the following sections:
  Overview of global AI development and important industries for application.
- Expectations for short, medium, and long-term technology development, including major stages, aims, and goals for AI in a certain country.
  The key challenges in developing AI technologies include identifying benefits, gaps, and development possibilities, as well as developing a plan of actions for technology development in general.
- The industry's financial assistance plans, as well as the implementation of specific AI technology initiatives, will be discussed.
  Topics covered include legal system adaptability, ethical challenges, and future technological advancement.
- Other examples:
  French strategy for artificial intelligence #FranceIA, France, 2018 Pan-Canadian Artificial Intelligence Strategy, Canada, 2018 New Generation of Artificial Intelligence Development Plan, China, 2017 National Strategy for Artificial Intelligence, Denmark, 2019.

Ethical papers:

AI regulation has traditionally focused on developing ethical papers to set application rules. By the end of 2019, there will be over 100 AI ethical statutes, guidelines, principles, and regulations worldwide. Typically, they address essential concepts including security, confidentiality, non-discrimination, and controllability. The Azilomari AI Principles, which were created in 2017, are a significant example. Other examples:

The Montréal Declaration on Responsible AI was published in 2017 and the Council of Europe Ad Hoc Group of High-Level Experts issued ethical recommendations for trustworthy AI in 2018. Model Convention on Robotics and Artificial Intelligence (2018) [38,39,40].

The significance of explain ability in developing reliable artificial intelligence for medical applications:

AI has the potential to tackle cognitive challenges that would otherwise need human intelligence, leading to significant advancement and innovation. AI has already made a significant impact on people's lives, including speech recognition, recommendation systems, and self-driving cars. AI is expected to become increasingly important in the future. The International Data Corporation predicts a rise in AI spending from 37.5 billion in 2019 to 97.9 billion in 2023[41]. AI has the potential to enhance people's health and well-being, especially with the growing availability of EHRs and other patient-related data. Examples include assisting professionals with diagnosis, identifying preventative possibilities, and offering individualized therapy suggestions. Some basic assisting technologies have been implemented in practice[42,43]. Creating explainable AI is one possible step toward trustworthy AI. Explainable AI seeks to understand how and why AI models make accurate predictions while retaining high performance levels[44]. Furthermore, the effectiveness of explainable AI systems needs to be shown in reality.

Conclusion

From the above rational, it can be suggested that the impact of Artificial Intelligence (AI) and Machine Learning in Pharmaceutical Sciences is significant and promising. AI technologies, through the analysis of large datasets, specialized hardware and software, and cognitive skills like learning and reasoning, are revolutionizing various aspects of pharmaceutical research and development. From drug discovery to personalized medicine and clinical trials, AI is enhancing efficiency, accuracy, and innovation in the pharmaceutical industry. As AI continues to evolve and be integrated into more pharmaceutical processes, it holds great potential for improving patient outcomes, reducing costs, and advancing medical science and health care system.

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