Review Article

Applications of Artificial Intelligence in Pharmaceutical Industries

Hansa Choudhary*[1], Anta Sharma[1], Dr. Dharmendra Ahuja[2]
[1]Student, Department of Pharmacology, Jayoti Vidyapeeth Women's University, Jaipur, Rajasthan, 303122, India.
[2]Dean, Department of Pharmacology, Jayoti Vidyapeeth Women's University, Jaipur, Rajasthan, 303122, India.
***Corresponding author's E-mail:** hansachoudhary55@gmail.com

Received: 19-04-2023; **Revised:** 24-06-2023; **Accepted:** 02-07-2023; **Published on:** 15-07-2023.

ABSTRACT

Artificial intelligence (AI) is used more and more in different societal fields, particularly in the pharmaceutical area. AI is advantageous from an economic and professional standpoint. By imitating human intelligence and combining it with cutting-edge technology to provide the best results, it minimizes the need for human work. This review examines the useful application of AI in the pharmaceutical industry at each stage from drug discovery through drug development as well as in several departments. In addition to requiring less human labor, it also enhances clinical research effectiveness and pharmaceutical productivity while decreasing the possibility of error. The review also looks at the current difficulties in implementing AI in the pharmaceutical industry. Additionally, it assesses current difficulties and suggests solutions.

Keywords: Artificial Intelligence, Drug development, Machine Learning, Pharmaceutical Industry.

QUICK RESPONSE CODE →

DOI:
10.47583/ijpsrr.2023.v81i01.027

DOI link: http://dx.doi.org/10.47583/ijpsrr.2023.v81i01.027

INTRODUCTION

The use of AI has grown globally across many industries. A review of its considerable impact on the pharmaceutical business is pending. Artificial intelligence (AI) is being used in a large numbers of pharmaceutical disciplines like medication research and development, medicine repurposing, accelerating pharmaceutical manufacturing, and clinical studies, which minimizes the amount of labor needed from humans while also advancing goals more quickly[1]. The difficulty of gathering, examining, and applying that knowledge to challenging healthcare scenarios has increased with greater digitalization[2]. This article examines the application of AI to several area of the pharmaceutical industry, from discovery of drugs to medication development. It includes utilizing AI to conduct clinical studies, repurposes drugs, increase pharmaceutical output, and more.

Artificial Intelligence

The usage of digitalization in the pharmaceutical industry has undergone significant development. The need for examination and trustworthy knowledge to address issues related to its acquisition and application in the field may be one of the hurdles that change always bring, nevertheless. These difficulties drive the inclusion of AI since it can manage massive data sets with improved automation. A modern technology-based system called artificial intelligence (AI) uses advanced tools, networking, and technologies to simulate human intelligence. It consists of hardware and software which can draw conclusions from the data provided and acts independently.

Computers are used in artificial intelligence to simulate intelligent decision-making. The most essential subsets of AI named as machine learning (ML), is commonly confused with AI. The term "machine learning" refers to the capacity to continuously statistically understand data without any explicit programming[3]. The use of AI could significantly change the speed and scope of drug discovery today. In general, the incorporation of AI in the pharmaceutical area can bring advancements such as:

- AI-based drug development doesn't rely on pre-established targets. As a result, during the medication development process, personal biases and previous experience are not taken into account.
- AI develops innovative algorithms for drug discovery by combining the most recent advances in biology and computation. Due to the rapid increase in processing power and decrease in processing costs, AI is having all what it takes to level up the levels of competition in drug research. AI has a higher capacity for defining pertinent interactions in pharmaceutical screens. Therefore, the likelihood of false positives can be reduced by carefully selecting the aforementioned test parameters.
- The capacity of AI to transform drug screening into a virtual lab, where promising targets can be reduced without demanding a lot of experimental input or

manpower hours, is perhaps its most important capability.

- The collection and storage of large amounts of digital patient data have become easier because of recent technological advancements. To help speed up the creation of novel medications and improve their chances of success in the early stages of development, AI platforms may mine the massive libraries of genomic information, health records, medical imaging, and other patient data[4].

Machine reasoning (MR) and AI

Machine reasoning (MR) is a fundamental subcategory of AI. MR makes use of learned information to navigate through a variety of options and get the optimal answer. To address some problems, deep subject knowledge is required, and MR is perfectly suited for this. A machine reasoner needs explicit human capture of all prior information to function on fresh input. MR is an excellent supplement to ML since it may analyze potential causes and improvement options in addition to extending the discoveries provided by ML[5].

Management of networks using AI and ML

Many challenges in network administration call for an immediate response. To solve these urgent issues, AI is being applied in four different areas of network administration. As follows:

- Traffic control,
- Performance evaluation,
- Capacity planning
- Security surveillance

Of all the AI techniques, ML is proven to be the most helpful in solving issues in the majority of these situations. AI is sophisticated enough to consider a wide range of potential fixes for several problems[5,6]. Examples include:

- Random optimization,
- Beam search,
- Simulated annealing,
- Blind hill climbing, and
- Optimization searches
- Calculations based on evolution
- Gene expression programming,
- Genetic programming,
- Genetic algorithms

Particle swarm optimization was inspired by the behavior of flocks of animals[7,8,9]

Logic

It can be used for expressing knowledge and solving problems, but it can also be used for other issues. For examples:

- The planning process in the SatPlan algorithm
- Probabilistic approaches to reasoning under uncertainty
- Case-based reasoning,
- AI research
- Logic of propositions
- uses truth-related operations like "or" and "not"
- Primate logic
- Predicates,
- Fuzzy,
- Default Logics,
- Non-Monotonic Logics,
- Propositional Logic,
- Adds Quantifiers,
- Fuzzy,
- Non-Monotonic Logics,
- Circumscription
- Non-monotonic logics,
- Default reasoning,
- The frame problem,
- Circumscription,
- The closed world assumption,
- Abduction
- The logic of description
- Displaying classes and relations[7]

Networks of artificial neurons

It was inspired from the structure of neuron in the human brain. Simple "neuron" N gets information via different "neurons," every one of which casts a weighted vote for or against whether neuron N should activate itself while active (or "fired"). A learning algorithm must be used to alter these weights in accordance with the training data[7]. Modern neural networks search for patterns in data and represent intricate relationships between inputs and results. They are capable of learning both digital logical processes and continuous functions. Since neural networks employ gradient descent to obtain access to a multiple dimensions topology that was constructed during training, they may be seen as a type of mathematical optimisation.

The backpropagation algorithm is the most widely used training method.

In-depth learning

The different layers can gradually pul upgraded information from the initial input. Lower layers in image processing, for instance, may recognize borders, whereas higher layers may recognize items that are significant to humans, such as numbers, characters, and faces connecting the network's inputs and outputs using an array of layers of neurons [9,10].

AI Application in the Pharmaceutical Industry

AI in Discovery of Drug

Drug development and research is a costly and laborious endeavor that necessitates balancing numerous features of molecules to achieve desirable clinical efficacy and safety. Among these characteristics, the drugs' performance primarily depends on their pharmacokinetics /pharmacodynamics (PK/PD) characteristics, nonclinical safety profiles, and absorption, distribution, metabolism, and elimination (ADME) characteristics. The discovery of drug and the process of its development may benefit from recent advancements in AI/ML techniques since they could increase the likelihood of success and speed up decision-making. Huge datasets that contain information about chemical structures and the associated experimental readouts are used to train the AI/ML system, which subsequently clarifies the underlying ideas, biological reactions, and interactions between chemical structures. The AI/ML models can then be used to predict the anticipated biological responses of a molecule that has not yet been tested and, in some circumstances, hasn't even been synthesized, only based on its chemical structure. To choose tiny compounds with the most potential ADME profiles for synthesis, testing, and process development, discovery scientists in the ADME sector employ these AI/ML models. These compounds are chosen from hundreds of thousands of theoretically possible options[11].

There are several uses of AI in drug discovery, and they can be categorized as follows:

a. Target validation and choice

Discovering the role of putative drug targets (genes/proteins of a small molecule) and their importance in illness requires understanding how these molecules work. The selection and validation methods must take into account functioning genomics, structure genomics, proteomics, in-vitro cell-based assays, and in-vivo animal research assays. AI evaluates the Drug Information Bank to ascertain the beneficial effects of drug candidates, genetic expressions, interactions between proteins, and clinical data records from a public library. To ascertain a drug's efficacy target, it is required to understand the function of potential molecular targets and their significance in illness.

b. Screening of compounds and lead optimization

To select drug candidates, compound screening and lead optimisation procedures combine virtual screening, high throughput screening, and combinatorial chemistry. To build the chemical database for AI-based virtual screening, significant amounts of compounds are retrieved from openly accessible chemogenomics libraries, which include millions of compounds with structural information.

c. Preclinical research

Preclinical studies, sometimes referred to as non-clinical studies, are laboratory tests conducted in vitro and in vivo on novel medicinal substances to ascertain their safety and efficacy profile. To quickly collect relevant huge amounts of biological data, clustering-based ML methods assess RNA sequencing technologies to discover a molecular mechanism of action. It also exposes several previously unknown relationships between different stimuli and the cytokines they affect.

d. Clinical Research

For recognizing patient conditions, finding gene targets, forecasting the outcome of a created drug, and on and off-targets, a generation of AI tools for clinical trials would prove excellent. In Phase II clinical studies, one AI mobile application boosted medicine adherence by 25% compared to conventional direct observation therapy[12].

AI IN DRUG SCREENING

The use of AI in drug screening includes target identification; molecular simulations; drug property predictions; de novo drug creation, synthesis of route generation, and candidate drug prioritization[12].

AI-based drug discovery tools and resources

Data resources are one of the fundamental elements of using AI for drug discovery and evaluation. Examples of data resources are ChEMBL, ChemDB, COCONUT, DGIdb, DrugBank, DTC, INPUT, PubChem, and SIDER or STITCH. Common AI methods include Delta Vina, neural graph fingerprint, alpha fold, and computer and additional techniques include clustering, classification, and regression analysis techniques[13,14].

AI in drug molecule design

Traditionally, designing a drug molecule requires a lot of effort and entails multiple failed attempts. For example, a synthesis plan can have hundreds of distinct steps, many of which would produce unfavorable byproducts or side effects or will just not work. AI, on the other hand, is now starting to enhance the efficiency of design, and synthesis, speeding up, streamlining, and lowering the cost of company operations while also reducing chemical waste[15]. In recent years, theoretical studies and research on AI (AI) have given way to actual implementations. Thanks to advancements in AI and ML techniques like deep learning (DL), machines may now imitate the intelligence of humans by learning from data. As a result, thanks to AI and ML

approaches, molecular design may see a revolution. Before AI, planning tests and characterizing, evaluating, and analyzing the findings of such investigations were almost completely the responsibility of specialists working in experimental laboratories that developed new substances. This bottleneck has slowed the creation of new materials, which could affect several sectors including electronics, medicinal development, and energy storage[16]. As a result of advancements in the field of computer science and the use of ML technology, many tools are now available. The possibility for considerably fewer computationally demanding simulations with sufficient precision for chemical applications is shown in quantum chemistry simulation utilizing ML techniques. ML applications include calculating stable structural conformations and producing coarse-grained models for molecular dynamics simulations. Inspiring research results have come from using ML to predict molecular characteristics. ML algorithms are now routinely used to predict features including the protein's reactivity, toxicity, and ability to bind to receptors from its electronic structure and amino acid backbone. This approach can be applied to chemistry to mimic the genesis of novel synthetic architectures. The development of synthetic molecular design with the aid of this technology could considerably boost chemical research[16].

AI is being used to develop new pharmaceutical products, including the following:

- Disease Identification/Diagnosis
- Personalized treatment with digital therapeutics and behavioral modification
- Drug Development and Production
- Prognostic forecasting
- Medical Tests

AI FOR PHARMACEUTICAL PRODUCTION

Manufacturing complexity has increased from prior years as a result of recent improvements in pharmaceutical technology and distinctive developments. For the complex procedure, a proven product's excellence and effectiveness are also necessary. Modern pharmaceutical production systems are striving to merge human expertise into machines to enhance manufacturing processes. The employment of AI in the production process has the potential to expand the pharmaceutical industry. Numerous pharmaceutical activities will be mechanized with the aid of AI tools. In addition to addressing problems that may occur during the manufacturing process, this can aid in numerical stimulation[17]. AI can be included in the manufacturing of medications to achieve the right level of outcomes by utilizing other cutting-edge manufacturing technologies. According to a discussion paper released by the U.S. FDA, the following potential applications of AI were seen in pharmaceutical production processes.

Process design and scalability: AI can quickly identify the processing parameters, reducing waste and development time.

Advance Process Control (ACP): When paired with real-time sensor data, AI can make it simpler to create process controls and, as a result, foresee how a process will develop. AI tools can recognize different maintenance approaches and equipment adjustments. This reduces downtime.

Trend detection: AI can be used to examine variations in customer feedback and complaints[18].

Although AI in pharmaceutical manufacturing can speed up and improve process efficiency, it's also important to consider how it will impact the equipment and infrastructure that are already in place.

AI for quality assurance and control

Pharmaceutical quality assurance and control systems are expected to benefit from the use of AI technologies. Bands are frequently used in the pharmaceutical industry to ensure that product quality requirements can be satisfied, although they aren't always as precise as they may be. The applications of AI in the pharmaceutical industry can predict even little variations that could have an impact on the functionality and safety of the products. Pharmaceutical quality control and assurance using AI can improve product quality and process accuracy[19]. However, the goods must go through manual quality control checks to maintain batch-to-batch homogeneity. Integration of AI could not be a workable strategy at this time. The Electronic Lab Notebook, a platform for automated data entry, along with cutting-edge AI algorithms, can assure product quality. It is feasible to adopt new technologies for intelligent quality control by using overall quality management expert systems, data mining, and other knowledge discovery techniques[17].

AI used in designing of Clinical Trials

Clinical trials are carried out to evaluate the efficacy and safety of drug items in humans for a particular disease condition. It could take 6-7 years or longer to complete this laborious process, and a sizable sum of money will also be required. Furthermore, the success rates are unacceptably low, which puts a significant burden on the industry. Failures may have a flawed patient selection strategy, poor infrastructure, or a lack of technical requirements as their underlying cause. Integration of AI can reduce this errors[17]. AI can carry out all stages of clinical trial design, including study preparation and study execution. This may increase trial success rates while easing the strain of pharmaceutical R&D. To obtain ethical and benchmarked results, the inclusion of AI in clinical trials must first be reviewed. The right strategy can reduce trial costs and failure rates while also speeding up the process[20]. AI can help in the selection of the population with specific illness conditions for Phase II and Phase III studies by using the patient-specific genome exposome profile analysis. The

preclinical discovery of compounds and the identification of the lead medications before to the initiation of clinical trials can both benefit from predictive ML, among other AI technologies.[17].

Pharmaceutical marketing

E-commerce and other marketing strategies are already utilizing AI in their successful marketing campaigns. Pharmaceutical companies can utilize comparable tools and techniques to expand and effectively serve their market. The tactics of AI in pharmaceutical marketing can greatly increase overall earnings.

Limitations of AI at the present moment

Despite all of the uses for AI in the pharmaceutical industry, there are some restrictions attached to it. To achieve the present standards of standard outcomes, AI must be developed. The demand for thorough training data for AI, which necessitates human labor and hence can have chances of inaccuracy, is one of the factors that indicate its limitations. As a result, AI integration is unavoidable. Another drawback of AI is that it can forecast models or structures via de novo medication creation, which is impossible to produce. A multidisciplinary strategy is needed to prepare healthcare workers for the use of AI because AI and ML are IT-based technologies, which may prove hard for the medical industry [21].

CONCLUSION

AI is increasingly integrating into our daily lives and becoming smarter with each passing day. This ensures its presence in every aspect of our existence. The use of AI in the pharmaceutical industry has the potential to revolutionize the industry, but its current state of development needs improvement. Given the limitations of current AI technology and the need for further research, it is still too early to predict if AI will have a significant impact on the pharmaceutical industry. The pharmaceutical industry has the potential to gain from AI because it has the potential to speed up and lower the cost of drug discovery while also improving clinical and pharmaceutical data through its cutting-edge technology. AI will benefit future generations, and pharmaceutical companies will also benefit from it. There are many obstacles and challenges related to this technology, hence there are currently no drugs on the market that were created utilizing AI approaches. Regardless of this, AI is likely to become a crucial tool for the pharmaceutical industry soon.

REFERENCES

1. Baran S, Henstock P. Pathways for Successful AI Adoption in Drug Development. SSRN. https://dx.doi.org/10.2139/ssrn.4305068
2. Ramesh AN, Kambhampati C, Monson JR, Drew PJ. Artificial Intelligence in Medicine. Annals of the Royal College of Surgeons of England. 2004; 86(5):334-7.
3. What is Artificial Intelligence in Networking? [Internet] 2023 [Cited 2023 June 4] Available from: https://www.cisco.com/c/en/us/solutions/artificial-intelligence/artificial-intelligence-machine-learning-in-networking.html#~q-a
4. Larranga P, Calvo B, Santana R, Bielza C, Galdiano J, Inza I, Lozano JA, Armanazas R, Santafe G, Perez A, Robles V. Machine learning in bioinformatics. Briefings in Bioinformatics. 2006;7(1):86-112.
5. AI & ML in Network Management. [Internet] 2023 [Cited 2023 June 4] Available from: https://www.comparitech.com/net-admin/ai-ml-in-network-management/ (accessed June 3, 2023).
6. Thakur A, Pokhriyal A, Gahlot D, Kukreti D. Human-Level Artificial Intelligence: One of the Future. IJRIT. 2014;2(9):373-9.
7. Froding B, Peterson M. Ethics and Information Technology. Friendly AI. 2021;23:207-14. https://doi.org/10.1007/s10676-020-09556-w
8. Nilsson NJ. Artificial Intelligence: A New Synthesis, Morgan Kaufmann Publishers 1998.
9. Mirmozafffari M, Yazdani R, Shadkam E, Khalili SM, Mahjoob M, Boskabadi A. An integrated artificial intelligence model for efficiency assessment in pharmaceutical companies during the COVID-19 pandemic. Sustainable Operations and Computers. 2022; 3:156-67.
10. Mishra V. Artificial Intelligence: the beginning of a new era in the pharmacy profession, Asian Journal of Pharmaceutics. 2018;12(2):18-23.
11. Why Artificial Intelligence Could Speed Drug Discovery. [Internet] 2022 [Cited 2023 June 7] Available from: https://www.morganstanley.com/ideas/ai-drug-discovery
12. How Artificial Intelligence is Revolutionizing Drug Discovery. [Internet] 2023 [Cited 2023 June 7] Available from: https://blog.petrieflom.law.harvard.edu/2023/03/20/how-artificial-intelligence-is-revolutionizing-drug-discovery/
13. Chen W, Liu X, Zhang S, Chen S. Artificial Intelligence for drug discovery: Resources, methods, and applications. Molecular Therapy – Nucleic Acids. 2023;31:691-702. https://doi.org/10.1016%2Fj.omtn.2023.02.019
14. Sima J, lee J, Wijaya L, Choi K, Coutlakis A. A literature review on the implementation of CRISPR systems and other biomedical tools on therapeutic interventions against tuberculosis. UC Berekeley Research Publications. 2022

15. Venkatraman S, Miah M. Artificial Intelligence in Healthcare: A Potential Fame Changer. Global Journal of Business Disciplines. 2022;6(1):56-9.

16. Artificial Intelligence in molecular design. [Internet] 2023 [Cited 2023 June 7] Available from: https://insights.globalspec.com/article/19909/artificial-intelligence-in-molecular-design#:~:text=AI%20can%20be%20used%20in,molecules%20and%20generate%20manufacturing%20processes

17. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discovery Today. 2019;24(3):773-780. https://doi.org/10.1016/j.drudis.2018.11.014

18. Using Artificial Intelligence & Machine Learning in the Development of Drug & Biological Products. U.S. Food & Drug. 2023

19. [Will AI Plan an Important Role in Quality Assurance and Quality Control Careers? [Internet] 2017 [Cited 2023 June 7] https://www.aaps.ca/blog/will-ai-play-an-important-role-in-quality-assurance-and-quality-control-careers

20. Henstock PV. Artificial Intelligence for Pharma: Time for Internal Investment. Cell Press. 2019;40(8):543-6.

21. Pareek V, Sharma L, Kumar S, Sharma V. Need for Artificial Intelligence in Pharmaceutical Industry and its Limitations. Journal of the Indian Academy of Geriatrics. 2022;18(14):217-20.

Source of Support: The author(s) received no financial support for the research, authorship, and/or publication of this article.

Conflict of Interest: The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.