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Artificial Intelligence in the Development and Discovery of Drugs

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Abstract

Artificial Intelligence (AI) had transfigured different sectors in society, where the pharmaceutical sector is not an exceptional case. Pharmaceutical sectors have reached new heights with the emergence of these sophisticated technologies. The evolution of artificial intelligence in the pharmaceutical industry is in a growth phase opening the possibilities of discovering many new drugs. The diseases affecting humans are increasing tremendously whereas the drugs which are available to treat or cure are very much minimal. But this kind of scenario will not be present in the future because of the combination of artificial intelligence and the pharmaceutical industry which results in faster discovery of drugs with increased clinical outcomes. The application of artificial intelligence caused a paradigm shift in the different phases of drug discovery. Artificial intelligence can shorten the time required for each step of the drug discovery process. Many pharmaceutical companies are using AI-based drug development techniques to treat a range of illnesses, including diabetes, Parkinson's disease, Alzheimer's disease, OCD, and more.

AI is also being used in product development to create nanorobots and nanomedicines. Only a few of AI-based medications are currently undergoing clinical trials, a sign of the growing field of AI-driven drug research. We have emphasized the use of AI in pharmaceutical product development and drug discovery in this review.

Keywords: Artificial Intelligence; Drug Discovery; Pharmaceutical Industry

Abbreviations: AI: Artificial Intelligence; ML: Machine Learning; DL: Deep Learning; ANNs: Artificial Neural Networks; FDA: Food and Drug Administration; NMSAC: National Manufacturing Strategy Advisory Committee; SACCAE: Strategy Advisory Center of the Chinese Academy of Engineering.

Introduction

The pharmaceutical industry has seen an enormous increase in the digitalization of data in the past few decades. But with digitalization also comes the difficulty of learning, examining, and using that information to deal with complicated clinical issues [1]. AI encompasses a number of approach domains, including knowledge representation, reasoning, and solution search, as well as a core machine learning paradigm (ML). Machine learning (ML) employs algorithms that identify patterns in a collection of data once it has been further categorized. Deep learning (DL), a branch of machine learning (ML), uses artificial neural networks (ANNs) [2]. The initial phase in the pharmaceutical business model is drug discovery, which entails finding novel therapeutic prospects. A drug candidate, which is the end product of the drug discovery process, is first put through preclinical research

and then developed into clinically relevant drugs. The safety, efficacy, dose, and tolerability of these drugs have been established by carefully planned and executed clinical trials. Drug discovery is an expensive, time-consuming, laborious, and frequently unsuccessful procedure. A chemical goes from the stage of discovery to the market in about 10 to 12 years.

History of AI

There has long been a theory that inanimate items could suddenly come to life and become sentient entities. Greek mythology featured robots and automatons created by Chinese and Egyptian engineers. The attempts of classical philosophers to characterize human thought as a symbolic system can be seen as the origins of current artificial intelligence. The term artificial intelligence (AI) was first used in 1956 at The Dartmouth Conference by American computer scientist John McCarthy. These days, it's a catch-all word that covers anything from real robotics to robotic process automation. Big data, or the growth in volume, velocity, and diversity of data that companies are currently gathering, has contributed to its recent rise in popularity. AI helps organizations get more information from their data by being more efficient than humans at things like finding patterns in the data.

Role of AI in Drug Discovery

There has been an important development in the methodology and efficacy of research in the fields of nanotechnology and personalized medicine. Incorporating automation and artificial intelligence (AI) aims to optimize drugs across many pharmaceutical industry sectors [3]. Followings are the role of AI in drug discovery system:

Artificial Intelligence can improve the Drug Discovery Process: Pharma companies are using artificial intelligence (AI) to help with the competitive and rather costly drug discovery process. Large datasets including disease patterns can be successfully identified by AI solutions, which can also assist in determining the optimal chemical compositions for treating various ailments [4]. As an illustration, consider the MIT-industry cooperation "Machine Learning for Pharmaceutical Discovery and Synthesis," which is made up of major players in the pharmaceutical business like Pfizer, Lilly, Bayer, and Novartis [5].

- Help efficiently access and analyze vast amounts of chemical data to ultimately improve business processes and outcomes.
- Provide critical insights into how to improve the designing, optimizing, and synthesizing of drugs.

AI Can Help in the Process of Drug Development and Production by making it More Effective: Artificial intelligence tools can improve the success rate of new drugs by:

- Performing quality control and ensuring high-quality standards
- Driving increased automation of daily core workflows
- Fixing supply chain issues within the production line and reducing wastage of materials
- Enhancing the production reuse value
- Performing predictive maintenance and reducing operational costs
- Forecasting demand and supply changes.

AI cans Provide Diagnostic Assistance and Empower Physicians to Deliver Personalized Treatment: At the heart of personalized treatment lies real-time patient data. AI-powered solutions and machine learning technology can empower healthcare brands to [6].

- Embrace a data-driven approach and analyse volumes of patient data
- Set up an electronic medical record system, whereby healthcare enterprises can store sensitive patient data on secure cloud platforms
- Drive customized treatment options in real-time by enabling doctors to look at historic patient data, previous diagnostic tests, etc.

Successfully diagnose issues. For instance, recently, the FDA authorized the marketing of an AI-drive platform-GI Genius-which can assist clinicians in detecting signs of colon cancer. This medical device leverages machine learning and AI algorithms to look for potential lesions in real-time during a colonoscopy.

Artificial Intelligence can Help Predict Epidemic Outbreaks:

Step 1: The AI/ML tools feed on real-time information that is gathered from disparate sources across the web.

Step 2: The predictive tool studies a multitude of environmental, biological, and other factors to make connections with previous epidemic outbreaks and provide relevant patterns, trends, and solutions.

AI can Enable Pharmaceutical Companies to 'Sell and Market' Better as Well as Smarter: Design out the customer journey, obtain real-time customer data, and gain insight into the needs, preferences, behavior, etc. of your customers superior. Develop original marketing plans that complement the commercial objectives of the organization and the specific needs of the target audience [7]. Analyze conversion rates, retention rates, and other key performance indicators to assess the effectiveness of marketing initiatives. Examine

past marketing campaigns and do a comparative analysis in order to identify any inefficiency in current strategy. It can also be used to forecast how successful marketing initiatives will be [8].

Industrial Applications: The new industrial revolution and the new technological revolution are known to be accelerating. We predict the arrival of a new era defined by omnipresent networks, data-drivenness, shared services, cross-border integration, automatic intelligence, and mass innovation—dubbed "Internet plus artificial intelligence (AI)." A crucial component of this new era is the rapid development and fusion of new AI technologies with Internet, new-generation information, new energy, materials, and biotechnology technologies. This will allow for the revolutionary transformation of models, means, and ecosystems with regard to their application to the national economy, well-being, and national security.

The foundation of the national economy, the means of subsistence for citizens, and national security is the industrial sector. An entirely new paradigm in manufacturing models, manufacturing processes, and its ecosystems is made possible by the profound merging of manufacturing technology with ICT, intelligent technology, and, above all, product-related expertise.

We consider intelligent manufacturing to be a new paradigm for manufacturing, as well as the technical means through which advanced manufacturing technology—such as design, production, management, testing, and integration—new information and communication technology, intelligent science and technology, large manufacturing technology, system engineering technology, and related product technology—are integrated with the entire system and lifecycle of product development. In order to enable the integration and optimization of various aspects of a manufacturing enterprise or group, including three elements (people/organizations, operational management, and equipment and technology) and five flows (information flow, logistics flow, capital flow, knowledge flow, and service flow), the manufacturing life cycle thus makes use of autonomous sensing, interconnection, collaboration, learning, analysis, cognition, decision-making, control, and the execution of human, machine, material, and environmental information [9,10].

Tools	Details	Website URL	Reference
Deep Chem	MLP model that uses a python-based AI system to find a suitable candidate in drug discovery	https://github.com/deepchem/deepchem	[11]
Deep Tox	Software that predicts the toxicity of total of 12 000 drugs	www.bioinf.jku.at/research/DeepTox	[12]
Deep Neural Net QSAR	Python-based system driven by computational tools that aid detection of the molecular activity of compounds	https://github.com/Merck/DeepNeuralNet-QSAR	[7]
ORGANIC	A molecular generation tool that helps to create molecules with desired properties	https://github.com/aspuru-guzik-group/ORGANIC	[13]
Potential Net	Uses NNs to predict binding affinity of ligands	https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	[14]
Hit Dexter	ML technique to predict molecules that might respond to biochemical assays	http://hitdexter2.zbh.uni-hamburg.de	[15]
Delta Vina	A scoring function for rescoring drug–ligand binding affinity	https://github.com/chengwang88/deltavina	[16]
Neural graph fingerprint	Helps to predict properties of novel molecules	https://github.com/HIPS/neural-fingerprint	[17]
Alpha Fold	Predicts 3D structures of proteins	https://deepmind.com/blog/alphafold	[18]
Chemputer	Helps to report procedure for chemical synthesis in standardized format	https://zenodo.org/record/1481731	[19]

Table 1: AI Tools Used in Drug Discovery.

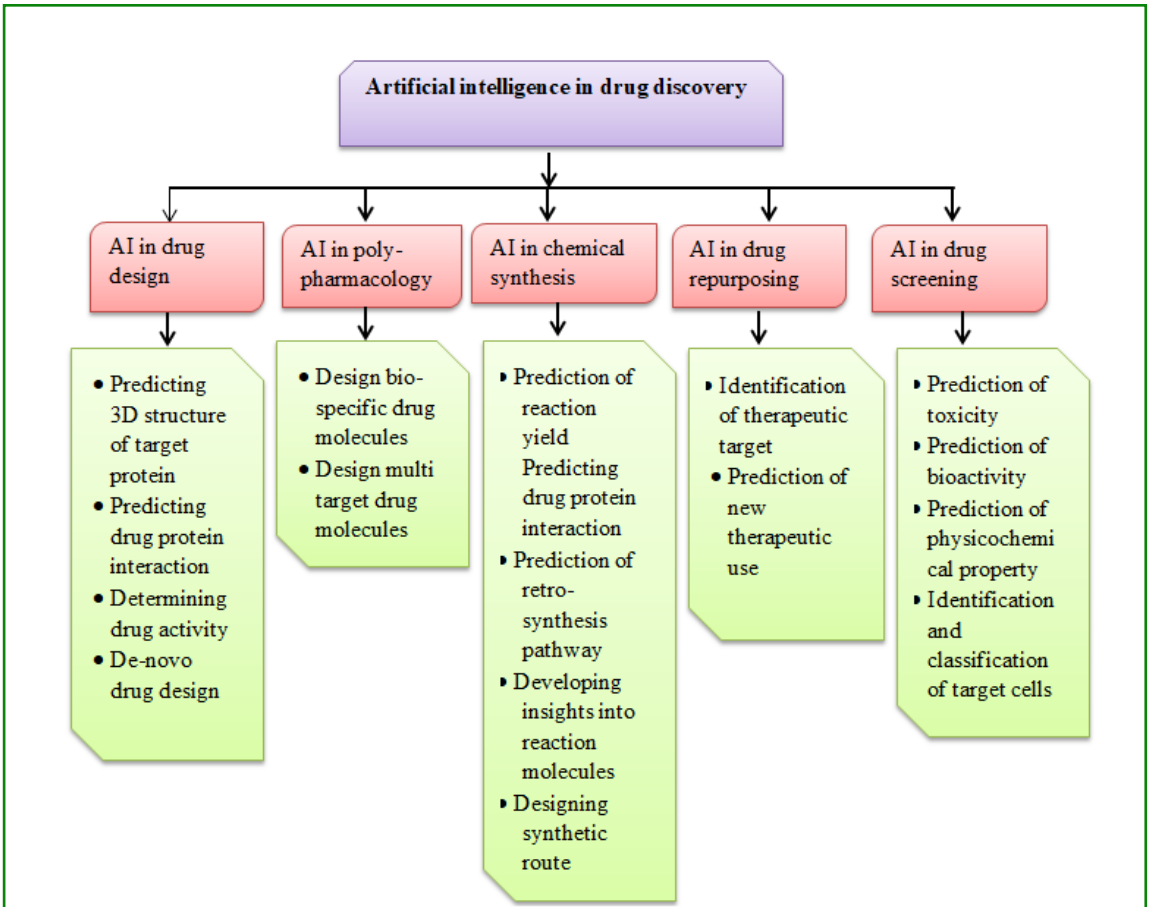

Figure 1: Role of AI in Drug Discovery.

Future Prospects

In India, artificial intelligence usage is encouraging. But for now, it's just getting started. While a few areas, like IT, manufacturing, the automotive industry, etc., are making use of AI's capabilities, its potential is still largely unexplored in many other fields.

The many additional technologies that fall under the AI category help to illustrate the enormous potential that AI possesses. Self-improving algorithms, machine learning, pattern recognition, big data, and many more are a few instances of these technologies. It is anticipated that this potent instrument would impact almost every business in the next years. This explains why India has enormous potential for the growth of AI.

In this comprehensive blog, we have discussed some of the sectors in which AI is being used: Artificial Intelligence is one of the most trending things right now. One can learn AI through various resources, whereas Intellipaat provides the AI Course in Bangalore in collaboration with IIT Madras.

Conclusion and discussion

AI's outstanding capabilities and ongoing advancements seek to lessen the obstacles faced by pharmaceutical companies, which could affect both the medication development process and the product's full lifetime. This could account for the rise in the number of start-ups in this industry. The rising cost of medications and treatments is only one of the many complicated issues the healthcare industry is currently facing. As a result, society needs to make some very big adjustments in this area. Artificial Intelligence (AI) can be used in pharmaceutical product manufacturing to create customized drugs with the right dose, release parameters, and other necessary elements based on each patient's needs [20]. Automation will become even more crucial as a result of the latest AI-based technologies, which will expedite the time it takes for products to reach the market while also improving product quality, safety throughout the production process, and cost-effective resource utilization [21]. The primary concern surrounding the integration of these technologies is the potential loss of jobs and the stringent laws required to integrate artificial intelligence. But these tools aren't meant

to fully replace people; rather, they're just meant to make tasks easier [22].

AI can also significantly aid in the optimization and continued integration of the developed medication in the appropriate dosage form. Furthermore, AI can facilitate prompt decision-making, which can expedite the production of higher-quality products and ensure batch-to-batch consistency. Through thorough market analysis and prediction, AI can also help prove the product's safety and efficacy in clinical trials and ensure appropriate placement and costing in the market. AI is not yet on the market, and there are still some obstacles to overcome before this technology can be widely used, but it is very likely that in the not too distant future, the pharmaceutical sector will find AI to be a very useful tool.

The phenomena of artificial intelligence (AI) and machine learning has been rapidly developing in recent years as researchers have discovered hundreds of potential applications for AI across a wide range of industries. In fact, to understand more about the most recent worldwide pandemic, scientists have begun employing AI and machine learning. This signifies the growing application of AI and machine learning together in the field of medicine research.

The epidemic has raised the need in the IT industry for AI and ML engineers. The need for jobs in AI and ML was least impacted by the nation's severe job losses. Companies are already moving toward expanding their work-from-home offerings, which will also call for experts in AI and ML. In conclusion, AI and ML have enormous promise, and a career in these fields can lead to significant advantages and in-demand employment.

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