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Artificial Intelligence In Drug Discovery And Development

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ABSTRACT

The importance of Computer Aided Drug Discovery (CADD) has been consistently increasing over the past 20 years. Artificial Intelligence (AI) is one of the CADD methods, machine learning (ML) is one of its subtopics. In the past five years , many Artificial Intelligence in Drug Discovery (AIDD) approaches were employed towards drug discovery . This article includes discussion on the scope and limitations of AIDD .

Artificial intelligence (AI) has been transforming the practice of drug discovery in the past decade. Various AI techniques have been used in many drug discovery applications, such as virtual screening and drug design. In this survey, we first give an overview on drug discovery and discuss related applications, which can be reduced to two major tasks, i.e., molecular property prediction and molecule generation. We then present common data resources, molecule representations and benchmark platforms. As a major part of the survey, AI techniques are dissected into model architectures and learning paradigms. To reflect the technical development of AI in drug discovery over the years, the surveyed works are organized chronologically. We expect that this survey provides a comprehensive review on AI in drug discovery. We also provide a G it Hub repository with a collection of papers (and codes, if applicable) as a learning resource, which is regularly updated.

Keywords:

Artificial intelligence, Computer-assisted drug discovery, Drug repositioning, Machine learning, DSP- 1181

INTRODUCTION:

Artificial Intelligence (AI) has recently started to gear-up its application in various sectors of the society with the pharmaceutical industry as a frontrunner beneficiary. This review highlights the impactful use of AI in diverse areas of the pharmaceutical sectors viz., drug discovery and development, drug repurposing, improving pharmaceutical productivity, clinical trials, etc. to name a few, thus reducing the human workload as well as achieving targets in a short period. Crosstalk on the tools and techniques utilized in enforcing AI, ongoing challenges, and ways to overcome them, along with the future of AI in the pharmaceutical industry, is also discussed. The use of artificial intelligence (AI) has been increasing in various sectors of society, particularly the pharmaceutical industry. In this review, we highlight the use of AI in diverse sectors of the pharmaceutical industry, including drug discovery and development, drug repurposing, improving pharmaceutical productivity, and clinical trials, among others; such use reduces the human workload as well as achieving targets in a short period of time. We also discuss crosstalk between the tools and techniques utilized in AI, ongoing challenges, and ways to overcome them, along with the future of AI in the pharmaceutical industry. Artificial Intelligence (AI) has recently started to gear-up its application in various sectors of the society with the pharmaceutical industry as a front-runner beneficiary. This review highlights the impactful use of AI in diverse areas of the pharmaceutical sectors viz., drug discovery and development, drug repurposing, improving pharmaceutical productivity, clinical trials, etc. to name a few, thus reducing the human workload as well as achieving targets in a short period. Crosstalk on the tools and techniques utilized in enforcing AI, ongoing challenges, and ways to overcome them, along with the future of AI in the pharmaceutical industry, is also discussed.

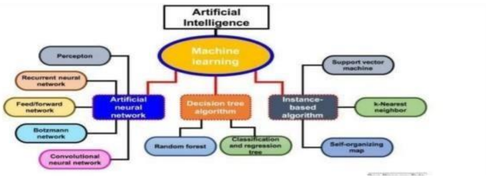
Artificial Intelligence:

Over the past few years, there has been a drastic increase in data digitalization in the pharmaceutical sector. However, this digitalization comes with the challenge of acquiring, scrutinizing, and applying that knowledge to solve complex clinical problems. This motivates the use of AI, because it can handle large volumes of data with enhanced automation. AI is a technology-based system involving various advanced tools and networks that can mimic human intelligence. At the same time, it does not threaten to replace human physical presence completely. AI utilizes systems and software that can interpret and learn from the input data to make independent decisions for accomplishing specific objectives. Its applications are continuously being extended in the pharmaceutical field, as described in this review. According to the McKinsey Global Institute, the rapid advances in AI-guided automation will be likely to completely change the work culture of society.

- **AI: Networks and Tools:**

AI involves several method domains, such as reasoning, knowledge representation, solution search, and, among them, a fundamental paradigm of machine learning (ML). ML uses algorithms that can recognize patterns within a set of data that has been further classified. A subfield of the ML is deep learning (DL), which engages artificial neural networks (ANNs). These comprise a set of interconnected sophisticated computing elements involving 'perceptions' analogous to human biological neurons, mimicking the transmission of electrical impulses in the human brain. ANNs constitute a set of nodes, each receiving a separate input, ultimately converting them to output, either singly or multi-linked using algorithms to solve problems. ANNs involve various types, including multilayer perceptron (MLP) networks, recurrent neural networks (RNNs), and convolutional neural networks (CNNs), which utilize either supervised or unsupervised training procedures.

The MLP network has applications including pattern recognition, optimization aids, process identification, and controls, are usually trained by supervised training procedures operating in a single direction only, and can be used as universal pattern classifier. RNNs are networks with a closed-loop, having the capability to memorize and store information, such as Boltzmann constants and Hopfield networks. CNNs are a series of dynamic systems with local connections, characterized by its topology, and have use in image and video processing, biological system modelling, processing complex brain functions, pattern recognition, and sophisticated signal processing. The more complex forms include Kohonen networks, RBF networks, LVQ networks, counter-propagation networks, and ADALINE networks. Examples of method domains of AI are summarized in figure. Several tools have been developed based on the networks that form the core architecture of AI systems. One such tool developed using AI technology is the International Business Machine (IBM) Watson supercomputer (IBM, New York, USA). It was designed to assist in the analysis of a patient's medical information and its correlation with a vast database, resulting in suggesting treatment strategies for cancer. This system can also be used for the rapid detection of diseases. This was demonstrated by its ability to detect breast cancer in only 60 s.



thus helping marketing executives to allocate resources for maximum market share gain, reversing poor sales andenabled them to anticipate where to makeinvestments. Different applications of AI in drug discovery and development are summarized in Figure 2

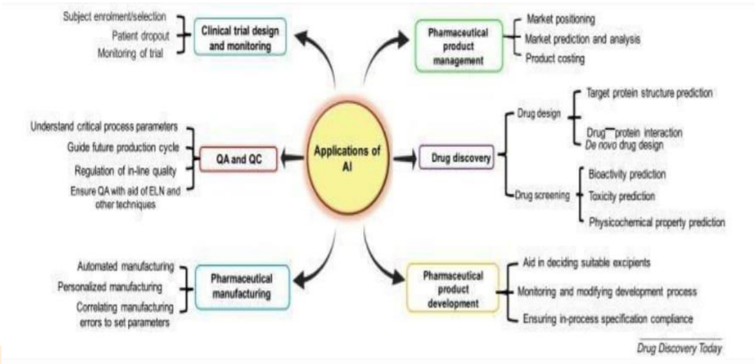


Figure 1 – Method Domains of AI

Figure 2 – Applications of AI

AI in lifecycle of pharmaceutical products:

Involvement of AI in the development of a pharmaceutical product from the bench to the bedside can be imagined given that it can aid rational drug design; assist in decision making; determine the right therapy for a patient, including personalized medicines; and manage the clinical data generated and use it for future drug development. E-VAI is an analytical and decision-making AI platform developed by Eularis, which uses ML algorithms along with an easy-to-use user interface to create analytical roadmaps based on competitors, key stakeholders, and currently held market share to predict key drivers in sales of pharmaceuticals,

Applications of AI:

AI in drug discovery:

The vast chemical space, comprising >1060 molecules, fosters the development of a large number of drug molecules. However, the lack of advanced technologies limits the drug development process, making it a time-consuming and expensive task, which can be addressed by using AI. AI can recognize hit and lead compounds, and provide a quicker validation of the drug target and optimization of the drug structure design. Different applications of AI in drug discovery are depicted in Figure 3.

Despite its advantages, AI faces some significant data challenges, such as the scale, growth, diversity, and uncertainty of the data. The data sets available for drug development in pharmaceutical companies can involve millions of compounds, and traditional ML tools might not be able to deal with these types of data. Quantitative structure-activity relationship (QSAR)-based computational model can quickly predict large numbers of compounds or simple physicochemical parameters, such as log P or log D. However, these models are some way from the predictions of complex biological properties, such as the efficacy and adverse effects of compounds. In addition, QSAR-based models also face problems such as small training sets, experimental data error in training sets, and lack of experimental validations. To overcome these challenges, recently developed AI approaches, such as DL and relevant modelling studies, can be implemented for safety and efficacy evaluations of drug molecules based on big data modelling and analysis. In 2012, Merck supported a QSAR ML challenge to observe the advantages of DL in the drug discovery process in the pharmaceutical industry. DL models showed significant predictivity compared with traditional ML approaches for 15 absorption, distribution, metabolism, excretion, and toxicity (ADMET) data sets of drug candidates.

QSAR modelling tools have been utilized for the identification of potential drug candidates and have evolved into AI- based QSAR approaches, such as linear discriminant analysis (LDA), support vector machines (SVMs), random forest (RF) and decision trees, which can be applied to speed up QSAR analysis. King et al. found a negligible statistical difference when the ability of six AI algorithms to rank anonymous compounds in terms of biological activity was compared with that of traditional approaches.

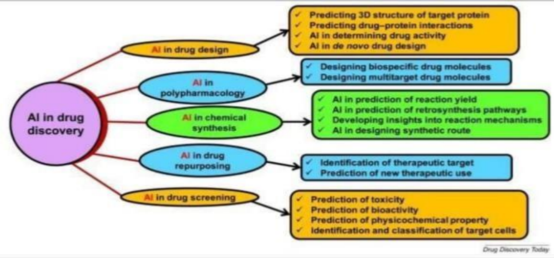


Figure 3 – Role of AI in drug discovery

1.3.2 AI in advancing pharmaceutical product development:

- The discovery of a novel drug molecule requires its subsequent incorporation in a suitable dosage form with desired delivery characteristics. In this area, AI can replace the older trial and error approach. Various computational tools can resolve problems encountered in the formulation design area, such as stability issues, dissolution, porosity, and so on, with the help of QSPR. Decision-support tools use rule-based systems to select the type, nature, and quantity of the excipients depending on the physicochemical attributes of the drug and operate through a feedback mechanism to monitor the entire process and intermittently modify it.
- Guo et al. integrated Expert Systems (ES) and ANN to create a hybrid system for the development of direct-filling hard gelatine capsules of piroxicam in accordance with the specifications of its dissolution profile. The MODEL EXPERT SYSTEM (MES) makes decisions and recommendations for formulation development based on the input parameters. By contrast, ANN uses backpropagation learning to link formulation parameters to the desired response, jointly controlled by the control module, to ensure hassle-free formulation development.
- Various mathematical tools, such as computational fluid dynamics (CFD), discrete element modelling (DEM), and the Finite Element Method have been used to examine the influence of the flow property of the powder on the die-filling and process of tablet compression. CFD can also be utilized to study the impact of tablet geometry on its dissolution profile. The combination of these mathematical models with AI could prove to be of immense help in the rapid production of pharmaceutical products.

1.3.3 AI in pharmaceutical product management:

A. AI in market positioning:

- Market positioning is the process of creating an identity of the product in the market to attract consumers to buy them, making it an essential element in almost all business strategies for companies to establish their own unique identity. This approach was used in the marketing of pioneer brand Viagra, where the company targeted it not only for the treatment of men's erectile dysfunction, but also for other problems affecting quality of life.

- With the help of technology and e-commerce as a platform, it has become easier for companies to get a natural recognition of their brand in the public domain. Companies exploit search engines as one of the technological platforms to occupy a prominent position in online marketing and help in the positioning of the product in the market, as also confirmed by the Internet Advertising Bureau. Companies continuously try to rank their websites higher than those of other companies, giving recognition to their brand in a short period.

B. AI in market prediction and analysis:

- The success of a company lies in the continuous development and growth of its business. Even with access to substantial funds, R&D output in the pharmaceutical industry is falling because of the failure of companies to adopt new marketing technologies. The advances in digital technologies, referred to as the 'Fourth industrial revolution', is helping innovative digitalized marketing via a multicriteria decision-making approach, which collects and analyses statistical and mathematical data and implements human inferences to make AIbased decision-making models explore new marketing methodology.
- AI also helped in a comprehensive analysis of the fundamental requirements of a product from the customer's point of view as well as understanding the need of the market, which aid in decision-making using prediction tools. It can also forecast sales and analyse the market. AI-based software engages consumers and creates awareness among physicians by displaying advertisements directing them to the product site by just a click. In addition, these methods use natural language-processing tools to analyse keywords entered by customers and relate them to the probability of purchasing the product.

AI in product cost

- Based on the market analysis and cost incurred in the development of the pharmaceutical product, the company determines the final price of the product. The critical concept in applying AI to determine this price is harnessing its ability to mimic the thinking of a human expert to assess the factors that control the pricing of a product after its manufacture. Factors, such as expenditure during research and development of the drug, strict price regulatory schemes in the concerned country, length of the exclusivity period, market share of the innovated drug after a year before are patent expiry, price of the reference product, and price-fixing policies determine the price of branded and generic drugs'

1.3.4 AI in Pharmaceutical manufacturing:

- The increasing complexities of manufacturing processes along with increasing demand for efficiency and better product quality, modern manufacturing systems are trying to confer human knowledge to machines, continuously changing the manufacturing practice. The incorporation of AI in manufacturing can prove to be a boost for the pharmaceutical industry. -Tools, such as CFD, uses Reynolds-Averaged Navier-Stokes solvers technology that studies the impact of agitation and stress levels in different equipment (e.g., stirred tanks), exploiting the automation of many pharmaceutical operations. Similar systems, such as direct numerical simulations and large eddy simulations, involve advanced approaches to solve complicated flow problems in manufacturing.
- The novel Champetre platform helps digital automation for the synthesis and manufacturing of molecules, incorporating various chemical codes and operating by using a scripting language known as Chemical Assembly. It has been successfully used for the synthesis and manufacture of sildenafil, diphenhydramine hydrochloride, and rufinamide, with the yield and purity significantly similar to manual synthesis. The estimated completion of granulation in granulators of capacities ranging from 25 to 600 can be done efficiently by AI technologies.
- The technology and neuro-fuzzy logic correlated critical variables to their responses. They derived a polynomial equation for the prediction of the proportion of the granulation fluid to be added, required speed, and the diameter of the impeller in both geometrically similar and dissimilar granulators.
- DEM has been widely utilized in the pharmaceutical industry, such as in

studying the segregation of powders in a binary mixture, the effects of varying blade speed and shape, predicting the possible path of the tablets in the coating process, along with analysis of time spent by tablets under the spray zone. ANNs, along with fuzzy models, studied the correlation between machine settings and the problem of capping to reduce tablet capping on the manufacturing line.

- Meta-classifier and tablet-classifier are AI tools that help to govern the quality standard of the final product, indicating a possible error in the manufacturing of the tablet. A patent has been filed, demonstrating a system capable of determining the most exquisite combination of drug and dosage regimen for each patient, using a processor receiving patient information, and designs the desired transdermal patch accordingly.

AI in Quality Control and Quality Assurance:

- Manufacturing of the desired product from the raw materials includes a balance of various parameters. Quality control tests on the products, as well as maintenance of batch-to-batch consistency, require manual interference. This might not be the best approach in each case, showcasing the need for AI implementation at this stage. The FDA amended the Current Good Manufacturing Practices (cGMP) by introducing a ‘Quality by Design’ approach to understand the critical operation and specific criteria that govern the final quality of the pharmaceutical product.
- Gams et al. used a combination of human efforts and AI, wherein preliminary data from production batches were analysed and decision trees developed. These were further translated into rules and analysed by the operators to guide the production cycle in the future. Goh et al. studied the dissolution profile, an indicator of batch-to-batch consistency of theophylline pellets with the aid of ANN, which correctly predicted the dissolution of the tested formulation with an error of <8%.
- AI can also be implemented for the regulation of in-line manufacturing processes to achieve the desired standard of the product. ANN-based monitoring of the freeze-drying process is used, which applies a combination of self-adaptive evolution along with local search and backpropagation algorithms. This can

be used to predict the temperature and desiccatedcake thickness at a future time point (t + Δt) for a particular set of operating conditions, eventually helping to keep a check on the final product quality.

- An automated data entry platform, such as an Electronic Lab Notebook, along with sophisticated, intelligent techniques, can ensure the quality assurance of the product. Also, data mining and various knowledge discovery techniques in the Total Quality Management expert system can be used as valuable approaches in making complex decisions, creating new technologies for intelligent quality control.

Clinical Trial Design:

- Clinical trials are directed toward establishing the safety and efficacy of a drug product in humans for a particular disease condition and require 6–7 years along with a substantial financial investment. However, only one out of ten molecules entering these trials gain successful clearance, which is a massive loss for the industry. These failures can result from inappropriate patient selection, shortage of technical requirements, and poor infrastructure. However, with the vast digital medical data available, these failures can be reduced with the implementation of AI.
- The enrolment of patients takes one-third of the clinical trial timeline. The success of a clinical trial can be ensured by the recruitment of suitable patients, which otherwise leads to ~ 86% of failure cases.
- AI can assist in selecting only a specific diseased population for recruitment in Phase II and III of clinical trials by using patient-specific genome–exposome profile analysis, which can help in early prediction of the available drug targets in the patients selected. Preclinical discovery of molecules as well as predicting lead compounds before the start of clinical trials by using other aspects of AI, such as predictive ML and other reasoning techniques, help in the early prediction of lead molecules that would pass clinical trials with consideration of the selected patient population.
- Drop out of patients from clinical trials accounts for the failure of 30% of the clinical trials, creating additional recruiting requirements for the completion of the trial, leading to a wastage of time and money. This can

be avoided by close monitoring of the patients and helping them follow the desired protocol of the clinical trial. - Mobile software was developed by Ai Cure that monitored regular medication intake by patients with schizophrenia in a Phase II trial, which increased the adherence rate of patients by 25%, ensuring successful completion of the clinical trial.

Pharmaceutical market of AI:

To decrease the financial cost and chances of failures that accompany VS, pharmaceutical companies are shifting towards AI. There was an increase in the AI market from US$200 million in 2015 to US$700 million in 2018, and is expected to increase to $5 billion by 2024. A 40% projected growth from 2017 to 2024 indicates that AI will likely revolutionize the pharmaceutical and medical sectors. Various pharmaceutical companies have made and are continuing to invest in AI and have collaborated with AI companies to developed essential healthcare tools. The collaboration of deep mind Technologies, a subsidiary of Google, with the Royal Free London NHS Foundation Trust for the assistance of acute kidney injury, is an example of this. Major pharmaceutical companies and AI players are detailed in Figure 4

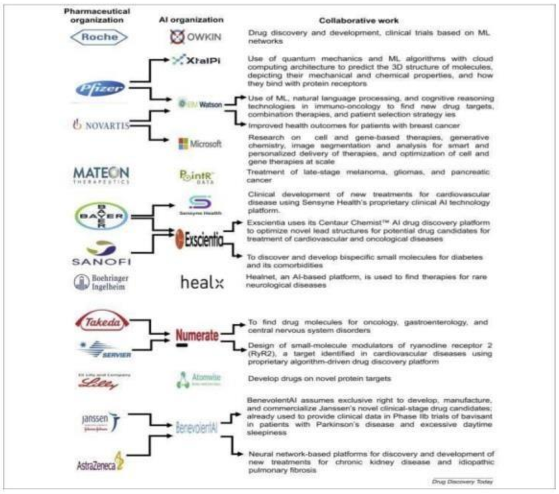


Figure 4 – Leading Pharmaceutical companies and their associations with AI

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AI based pharmaceutical start-up companies:

- According to Emersion Insights research, AI start-ups in drug development raised about 2.1 billion USD in the first half of 2021.
- AI is already been used by big biopharmaceutical companies at

various stages of drug discovery. For example, Pfizer is using IBM Watson, a machine learning-based system to search for immuno-oncology drugs. Roche Geotech is using GNS healthcare from Cambridge, Novartis is using Microsoft for research on cell and image segmentation, and AstraZeneca is associated with Benevolent to develop and commercialize Jenssen's novel clinical stage candidates.

- Companies like Google, DeepMind, Insilco Medicine, Deep Genomics, heal etc., are also making huge investments in AI-based drug discovery applications. In this Section, we discuss recent developments and prominent AI-based companies for drug development.
- USA is the pioneer and the dominant participant in AI implementation and hosting more than half of the world's AI companies for drug discovery businesses. A huge increase in the number of investors in the USA and the European Union has been observed in recent years. As a result, these areas, along with the United Kingdom, are the leaders in terms of the number of investors in AI-based drug discovery applications.
- Novartis is a major player in the pharmaceutical AI race in the United Kingdom and the European Union. Benevolent AI and AstraZeneca, two UK-based companies, are working together on a novel AI-generated chronic kidney disease target. Recently, China is also focusing on investment in AI for drug discovery and it has vowed to invest US $5 billion in AI. Tianjin, one of China's largest cities, will invest US $16 billion in its AI business, while Beijing will create a $2.12 billion AI development project. By 2030, China envisions becoming the leader in AI-based drug discovery start-ups.
- As shown in Fig. 5, the USA is the leading country with 55.10% companies, followed by Europe and the UK with 19.90% and 9.95% proportion in the adoption of AI-based solutions for drug discovery. Meanwhile, Asia currently has the fourth-lowest proportion in the adoption of AI-empowered drug discovery start-ups.

Figure 5 – Statistics of AI Start-ups for drug discovery

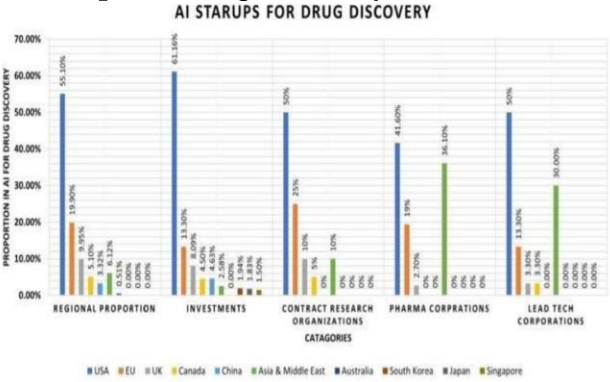

Figure 5 – Statistics of AI Start-ups for drug discovery

- USA also leads the AI race in terms of Contract Research Organizations (CRO), with 50% of CROs situated in the United States followed by Europe which has 25% CROs. Meanwhile, Asia also has 10% CRO interested in AI-oriented drug discovery. According to the number of IT companies using AI in healthcare and drug research, the United States leads all the countries.
- However, in terms of the number of chemical corporations, Asia has the second highest number, with the EU in third place. This makes sense in light of the EU's recent growth in the chemical sector, which now outnumbers the US and Asian markets for chemical compounds and related goods.

Case studies of successful AI - aided drug discovery efforts:

The potential of AI in the context of drug discovery has been demonstrated in several case studies. For example, the successful use of AI to identify novel compounds for the treatment of cancer has recently been reported by Gupta, R., et al. These authors trained a DL algorithm on a large dataset of known cancer-related compounds and their corresponding biological activity. As an output, novel compounds with high potential for future cancer treatment were obtained, demonstrating the ability of this method to discover new therapeutic candidates. The use of ML to identify small-molecule inhibitors of the protein MEK has recently been described. MEK is also a possible target for the treatment of cancer, but the development of effective inhibitors has been challenging. The ML algorithm was able to identify novel inhibitors for this protein. Another example is the identification of novel inhibitors of betasecretase (BACE1), a protein involved in the development of Alzheimer's disease by using an ML algorithm. AI has also been successfully applied in the discovery of new antibiotics .A pioneering ML approach has identified powerful types of antibiotic from a pool of more than 100 million molecules, including one that works against a wide range of bacteria, such as tuberculosis and untreatable bacterial strains .The use of AI in the discovery of drugs to combat COVID-19 has been a promising area of research during the last two years .ML algorithms have been used to analyse large datasets of potential compounds and identify those with the most potential for treating the virus. In some cases, these AI-powered approaches have been able to identify promising drug candidates in a fraction of the time that it would take when using traditional methods. Many more examples are available , showing that AI-based methods can accelerate the drug discovery process and enable the development of more effective medications.

Challenges and Limitations of using AI in drug discovery:

- Despite the potential benefits of AI in drug discovery, there are several challenges and limitations that must be considered. One of the key challenges is the availability of suitable data.
- AI-based approaches typically require a large volume of information for training purposes. In many cases, the amount of data that is accessible may be limited, or the data may be of low quality or inconsistent, which can affect the accuracy and reliability of the results. Another challenge is presented by ethical considerations since AI-based approaches may raise concerns about fairness and bias (see next section).
- For example, if the data used to train an ML algorithm are biased or unrepresentative, the resulting predictions may be inaccurate or unfair. Ensuring the ethical and fair use of AI for the development of new

therapeutic compounds is an important consideration that must be addressed.

- Several strategies and approaches can be used to overcome the obstacles faced by AI in the context of chemical medicine.

Ongoing challenges in adopting AI:

- The entire success of AI depends on the availability of a substantial amount of data because these data are used for the subsequent training provided to the system. Access to data from various database providers can incur extra costs to a company, and the data should also be reliable and high quality to ensure accurate result prediction.
- Other challenges that prevent full-fledged adoption of AI in the pharmaceutical industry include the lack of skilled personnel to operate AI-based platforms, limited budget for small organizations, apprehension of replacing humans leading to job loss, scepticism about the data generated by AI, and the black box phenomenon (i.e., how the conclusions are reached by the AI platform).
- Automation of certain tasks in drug development, manufacturing, and supply chains, clinical trials, and sales will take place with time, but these all fall under the category of 'narrow AI'; where AI has to be trained using a large volume of data and, thus, makes it suitable for a particular task. Therefore, human intervention is mandatory for the successful implementation, development, and operation of the AI platform. However, the fear of unemployment could be a myth given that AI is currently is taking over repetitive jobs, while leaving scope for human intelligence to be used for developing more complicated insights and creativity.
- Nevertheless, AI has been adopted by several pharmaceutical companies, and it is expected that a revenue of US$2.199 billion will be created by 2022 through AI-based solutions in the pharmaceutical sector, with an investment exceeding US$7.20 billion across 300+ deals between 2013 and 2018 by the pharmaceutical industry.
- Pharmaceutical organizations need clarity about the potential of AI technology in finding solutions to problems once it has been implemented, along with understanding the reasonable goals that can be achieved. Skilled data scientists, software engineers with a

sound knowledge of AI technology, and a clear understanding of the company business target and its R&D goal can be developed to utilize the full potential of the AI platform.

RATIONAL OF WORK:

Aim: A Review on the use of Artificial Intelligence in Drug Discovery & Development.

Objective:

1. Artificial Intelligence (AI) has revolutionized many aspects of the pharmaceuticals.
2. AI assistance to pharma industries helps to improve overall life cycle of product.
3. AI can be implemented in pharma ranging from drug discovery to product management.
4. Future challenges related to AI and their respective solutions have been expounded.

LITERATURE REVIEW:

1. Lamberti M.J, et al (2019).: - Mary Jo Lamberti studied on the application and use of artificial intelligence to support drug development. The Tufts Centre for the Study of Drug Development (CSDD) and the Drug Information Association (DIA) in collaboration with 8 pharmaceutical and biotechnology companies conducted a study examining the adoption and effect of artificial intelligence (AI), such as machine learning, on drug development. A 2-part method was used that comprised in-depth interviews with AI industry experts and a global survey conducted across pharmaceutical and biotechnology organizations. The study revealed that the significant challenges to AI implementation includes staff skills, data structure and budgets.

2. Bielecki A., et al, (2019): - Andrzej Bielecki is a Polish scientist who studied in AGH University of Science and Technology. The first stage of studies concerning the computer analysis of hand X-ray digital images is described. The images are pre-processed and then skeletisation of the fingers is carried out. Then, the interphalangeal and metacarpophalangeal joints are detected and contoured. Joint widths are also measured. In recent years wind energy is the fastest growing branch of the power generation industry. The largest cost for the wind turbine is its maintenance. A common technique to decrease this cost is a remote monitoring based on vibration

analysis. These were the studies of Andrzej Bielecki.

3. Mak K.-K., Pichika M.R. et al, (2019): - Mak and Pichika both have a very big contribution in the field of Artificial Intelligence. They worked on the present status and future prospects in the drug development. The study of machine learning in drug discovery and development for the future prospects was important.

4. Gams M, et al, (2014): - Matjaz Gams is a Slovenian computer scientist and researcher in artificial intelligence at Department of Intelligent systems, Jožef Stefan Institute, Ljubljana, member of the National Council of the Republic of Slovenia, its councillor for science and research, and member of AAAI, IEEE and ACM. He has a great contribution in Ambient Intelligence and Artificial Intelligence. Ambient intelligence (AmI) is intrinsically and thoroughly connected with artificial intelligence (AI). Some even say that it is, in essence, AI in the environment. AI, on the other hand, owes its success to the phenomenal development of the information and communication technologies (ICTs).

5. Aksu B, et al, (2013): - Buket Aksu worked on quality by design approach using artificial intelligence techniques to control the critical quality attributes of ramipril tablets manufactured by wet granulation. Quality by design (QbD) is an essential part of the modern approach to pharmaceutical quality. The study was conducted in the framework of a QbD project involving ramipril tablets. Preliminary work included identification of the critical quality attributes (CQAs) and critical process parameters (CPPs) based on the quality target product profiles (QTPPs) using the historical data and risk assessment method failure mode and effect analysis (FMEA).

SUMMARY AND CONCLUSION:

AI-based methods are being adopted in the health care industry where low-cost, intelligent, and flexible methods are affecting areas such as drug design, support for clinical decision making, diagnosis, prevention, and making clinical recommendations. AI applications were previously thought to be inferior to experimental high-throughput screening, combinatorial chemistry, and other technical drivers. It was difficult to create new chemical entities using computer programs, with desired features from the ground up, potentially even better than a human expert. The long and costly process of drug design can be accelerated by employing data science methods for target identification, De novo molecular design, drug repurposing, retrosynthesis and prediction of reactivity and bio-activity, FDA approval, and post-market analysis. AI has been implemented by some pharmaceutical organizations, with revenue from AI-based solutions in the pharmaceutical sector estimated to reach US $2.199 billion by 2022. Deep neural networks (DNNs) can be used to boost prediction power when inferring the properties of small molecules, and one-shot learning can be used if a large amount of experimental data is not available. Understanding technical and human errors, labelling constraints, and biological variability associated with the underlying data is crucial to create useful predictive models. It is difficult to represent the experimental data in numerical or computer-assisted form. AI is now being utilized to create representations of trials that allow for data categorization and, ultimately, the development of predictive models.

FUTURE SCOPE:

Like industry, regulators can employ AI to improve processes. In fact, FDA currently uses AI for translating documents, screening adverse event reports, and forecasting the volume of incoming regulatory submissions. In the future, both manufacturers and regulators might benefit from the extensive data and analysis provided by the expanded use of AI. International regulators have projected using AI to detect false or misleading drug information, scan scientific literature, identify safety signals, and respond to public inquiries.

While there are potential benefits of AI, there are also risks. Access to high-quality data is a fundamental requirement for effective AI training or learning. AI can be particularly sensitive to the characteristics of the data used for training, testing, and validation. The process analytical technologies providing data to AI systems must be accurate and representative. For learning purposes, data must represent not only process successes but also process failures. It will be critical to ensure that data used for AI training or learning are fit for use based on quality, reliability, and representativeness.

Humans, and not machines, are ultimately responsible for assuring that high-quality drugs are available to patients. Humans must be able to interpret the information generated by AI enough to ensure, for example, adherence to current good manufacturing practice requirements. Yes, AI has the potential to significantly improve pharmaceutical manufacturing.

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