ROLE OF ARTIFICIAL INTELLIGENCE IN BIOTECHNOLOGY TO DESIGN AND DEVELOP A DRUG: A REVIEW

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ABSTRACT

The term "artificial intelligence" (AI) refers to a set of technologies that have come together to mimic the four main aspects of human intelligence: perception, cognition, action, and learning. The process of developing new medicines is complex and time-consuming, but AI is making it simpler and less expensive. Machine learning (ML) is used to extract insights from large amounts of diverse data to create decision-supporting predictive models in the pharmaceutical industry. AI is being used to model disease heterogeneity, identify therapeutic targets, design and optimize drugcandidates, and predict in silico their clinical efficacy. Thus, by bolstering the justification for the selection of target and therapeutic candidates, the drug development process will be able to proceed more quickly and with fewer setbacks. Medication target recognition evidence, sedative screening, image screening, and predictive demonstrating are just a few examples of how AI is being put to use in the biotech industry. Similarly, AI is being used to organize preliminary clinical data and analyse rational writing. Artificial intelligence (AI) has been explained in detail throughout this assignment, along with its various processes, procedures, applications, and usage in the biotechnology industry.

Keywords: Drug, Biotechnology, Artificial Intelligence.

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1. INTRODUCTION

The ability of technologies like computers and robots to do activities that have historically required human knowledge and judgement is what we mean when we talk about artificial intelligence (AI). The introduction of a novel drug molecule into clinical practice is known as drug development. Several tasks throughout drug discovery and development have benefited from the application of AI, including the identification of new targets [1], an increase in understanding of disease mechanisms, and the creation of novel biomarkers. The pharmaceutical business has started investing in resources, technology, and services to enhance artificial intelligence (AI) research in fields including machine learning and deep learning. The illustration is given in Figure 1.

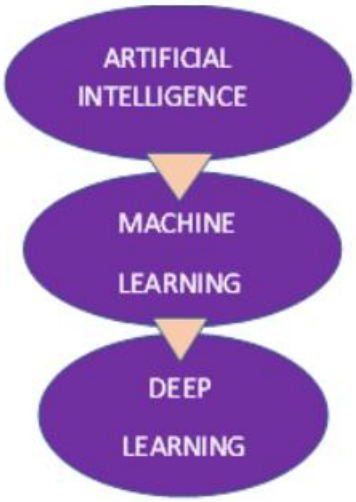

Figure 1: Learnings for drug development

There is now a substantial role for AI in pharmaceutical research, and several companies have either created in-house AI initiatives or partnered with external AI companies to do so. Artificial intelligence is currently being employed by some companies to find new applications for existing medications and late-stage medicinal possibilities. Therapeutic development refers to the overall effort to bring a novel drug

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molecule to clinical use. Everything from discovering the right molecular target to carrying out massive Phase III clinical trials in preparation for a drug's commercial release falls under this category. AI computational docking (s) often involve the generation, scoring, and comparison of a new posture to one that has previously been used. When it comes to docking a molecule to a target in virtual screening, there are a few different docking systems to choose from. Each one has its sampling methods, scoring algorithms, ligand and receptor flexibility treatment, and computing time requirements.

Though the term "artificial intelligence" (AI) may conjure images of the future, it is already at work in a wide range of commonplace technologies. It enables speech and face recognition on our portable devices, for instance. Artificial intelligence is also having an effect in the biotechnology sector, where it is rapidly becoming indispensable in many areas of drug discovery and development. Artificial intelligence (AI) can handle unique clinical preliminary datasets, perform virtual screening, and analyze enormous data sets. Artificial intelligence (AI) has the potential to reduce clinical preliminary costs [1-5] and enhance seemingly meaningless pieces of information, which could then be fed back into the drug development process.

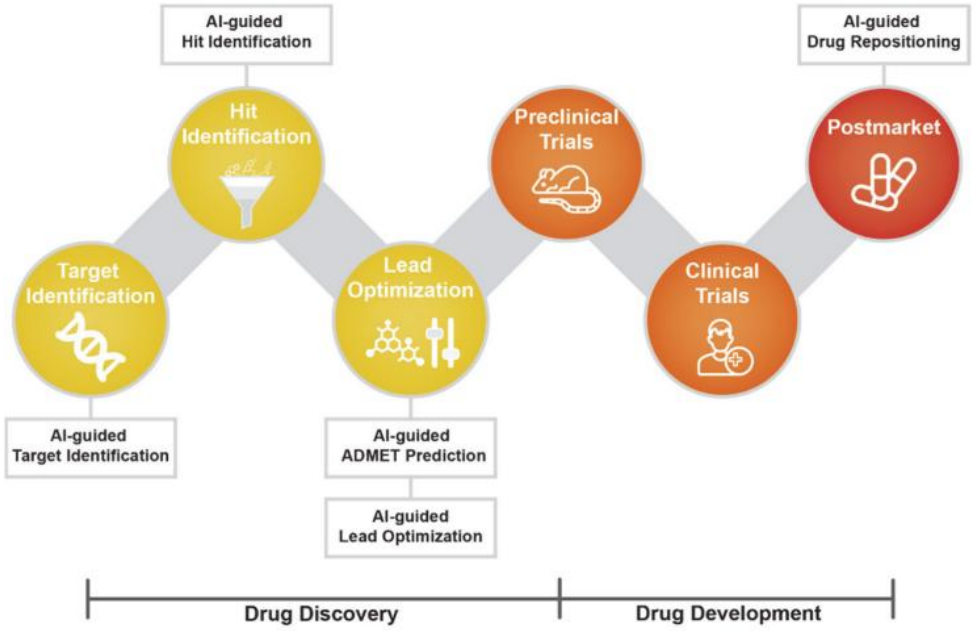

Fig. 2. The entire procedure for creating new drugs. With the help of AI tools, the drug development dropout rate can be lowered, and this is primarily done during the drug discovery phase. The associated methodology presents the areas of drug discovery that are relevant to AI applications.

Recent data-driven research developments in areas that can benefit from artificial intelligence to a significant extent (such as those involved in the drug discovery process) are the subject of this review. Aiming, Hitting, Optimising Leads, and Following Up After the Sale (Fig. 2). Cutting-edge AI technology and the potential of big data bring substantial benefits when used in the aforementioned stages of drug discovery.To begin the process of discovering less biased and novel drugtargets, we can examine connected multi-omics and linkage data in search of data-driven patterns that are difficult for humans to extract. Second, we may drastically cut down on the time and money spent on experimental validation by virtually screening a large number of compounds using rapid and

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reliable predictive models. Finally, researchers can find the best way to continue optimizing leads thanks to the novel optimized candidate structures that can be developed and evaluated by AI models. Last but not least, the commercially available medications that are suggested as promising off-targets by AI will result in substantial cost reductions. Given this, we analyze the present developments in each subject and explore the existing limitations of AI applications therein, before making recommendations for the way forward.

2. LITERATURE REVIEW

Over the past two decades, pharmacists and biologists have faced a formidable challenge: how to design cutting-edge systems for the safe and effective delivery of therapeutic drugs to specific areas of the body. [1].

Another drawback of medication design and development was the time and money required to create innovative therapeutic agents [2].

The scientific community all across the world has turned to computational methods like molecular docking and virtual screening (VS) to help them deal with these challenges. However, limitations such as accuracy and efficiency are inherent to these methods [3].

This has led to a rise in the use of cutting-edge methods that can function independently of more conventional computing strategies. It is possible that artificial intelligence (AI), and more specifically deep learning (DL) and machine learning (ML) algorithms, can help researchers find effective ways to work around problems that arise throughout the drug discovery process [4].

Target identification and validation, therapeutic screening, lead compound optimization, preclinical and clinical trials, and manufacturing are just a few of the many time-consuming activities involved in drug development and design. All of these requirements represent a significant barrier to finding a cure for a disease. Therefore, pharmaceutical companies' primary concern is controlling the cost and speed of the procedure [5].

Artificial intelligence (AI) has provided straightforward, evidence-based solutions to all these concerns, drastically cutting down on both the time and money required to complete the process. In addition, the rise of digital data in the healthcare industry and pharmaceutical businesses drives the use of AI to solve the difficulties of analyzing complicated data [6].

Artificial intelligence, or AI, is defined as the capacity of machines to acquire knowledge and improve their performance via observation and experience. Using AI is defined as "cognitive behavior in a machine that is typical of the human brain in learning and problem solving" [7].

These days, AI algorithms are being heavily incorporated into the medication design and discovery process by both biological and chemical researchers [8].

Computational modeling based on AI and ML concepts can substantially assist in the assessment of toxicity and physiochemical property evaluation, drug monitoring, drug efficacy and effectiveness, and drug repositioning [9].

AI principles combined with ML and DL algorithms have made VS of substances from chemical libraries, which include over 106 million compounds, easy and efficient. In addition, AI models eliminate the risks of non-intended toxicity [10].

This paper provides a high-level overview of the growth of artificial intelligence (AI) from ML to DL, as well as the role that big data has played in the revolution in the drug discovery process. We then talked about how AI is being used to improve traditional drug development and how combining AI with traditional

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chemistry is helping to improve the drug discovery process. Then, we talk about how AI is used at different points in the drug development process, such as during primary and secondary screening, toxicity testing, drug release, and monitoring, finding the optimal dose, repositioning drugs, dealing with polypharmacy, and figuring out drug-target interactions.

3. ROLE OF ARTIFICIAL INTELLIGENCE IN BIOTECHNOLOGY

A small number of companies are developing AI technologies to support the biotech sector. As more time-consuming methods like traditional quantifiable testing or manual photo checking reach their limits, their services are fast becoming essential [11]. Normal methods of data examination in quiet revelation are most effective when dealing with simple, consistent data. However, when the information becomes complex, such as when patient records contain a wide variety of findings, commodities, complex treatment plans, and numerous experiences across a wide range of facilities and providers, these methods fall short. Sensyne Health has been at the forefront of this development in clinical data [12]. Rabia T. Khan, Ph.D., head of translational medicines at Sensyne, claims that the typical approach to medication disclosure is impractical because it wastes billions of dollars and still generates high disappointment rates. However, she does point out AI's potential to cut down on expenses and disappointments. Sensodyne is collaborating with the NHS to better understand patients and better define them for clinical preliminary work.

She believes that eventually, businesses will shift their focus from physical to digital preliminary testing. With the use of artificial intelligence, virtual preliminary examinations will provide a large portion of the data that previously required expensive human preliminary examinations. This information will be made available for a future drug well in advance of any human testing. Instead of developing a notion in a petri dish and then testing it on humans, Khan's biotech firm will begin with real-world data, interface it with persistent examples, and utilize it to find new tranquilizers; we will then care for the same data again in the clinical trial.

3.1 Example of Biotechnology industry using AI technique

Precision Medicine Group is another group that focuses on monitoring clinical preliminary data. QuartzBio, an artificial intelligence platform, was recently acquired by the company's Precision for Medicine division [13]. This platform processes natural and clinical data streams to extract insights and knowledge that can be used to develop medicines more quickly. According to Precision Medicine Group's senior vice president, Cliff Culver, this strategy is only seldom fruitful. "Every last bit of that data is generated independently and exists in isolated designs all around the world," he explains. "For a pharmaceutical company, arranging all of that would require the combined efforts of numerous people over weeks or months, especially if the core involves linking measurable'reportable' back to source data (such as images or sequencing information) to enable ongoing quality control. "The outcome is that investigation is definitively postponed, regularly until after a preliminary is finished. What's more, there's a once-in-a-while transmission capacity to embrace profound information combinations across preliminaries inside an association. We do it as a preliminary is unfurling, so the organization has standard knowledge into what's going on, and afterward, we do it at a venture level to augment the utility of the information." QuartzBio's unsupervised artificial intelligence testing resembles that of

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Google, Netflix, and other digital giants in several ways. In any event, selecting a movie you'll enjoy is much more like finding organic bits of knowledge.

3.2 On-the-fly Examinations Advancement

The Concerto Health AI team specializes in oncology and is a precision pharmaceutical firm. Artificial intelligence is used to learn about how medications work in practice. The group's efforts have the potential to standardize the pharmaceutical research process, instruct in the ways of results exploration and value-based investigations, and speed up the sedative turnaround. Researchers in the field of biotechnology have access to a vast trove of data; as a result, it's becoming increasingly important for them to rely on computerized reasoning and artificial intelligence to make sense of it all, finish their data analysis projects on time, and make meaningful progress. Agricultural biotechnology, clinical biotechnology, animal biotechnology, mechanical biotechnology, and bioinformatics are all subfields within the larger field of biotechnology. Let's take a look at the influence that AI is having on this subfield of biotechnology [14].

3.3 Medical Biotechnology

To improve human health, medical biotechnology employs living cells to transport therapeutics and antidotes. It also involves studying DNA and cellular inheritance to enhance the production of useful and important properties. The fields of sedate revelation and Artificial Intelligence (AI) consciousness and Machine Learning are both highly utilized. Artificial intelligence aids in locating minute particles that, depending on the actualized objective structures, may provide beneficial therapeutic effects [15]. Artificial intelligence is commonly used in disease diagnosis because it learns from the actual result to refine the analytical tests; in other words, the more illustrative tests that are performed, the more precise the results may be. Radiation therapy planning is another area where AI is helping to make a positive impact by cutting down on time spent on administrative tasks to better prioritize each patient's needs. Improving electronic health records (EHRs) with evidence-based medications and clinical choice emotional support networks is another area where AI and ML are showing signs of promise. In addition to the aforementioned fields, these technologies are widely used in quality assurance, radiography, personalized medicine, healthcare administration, and many more. Table 1 summarises the many artificial intelligence tools that have been implemented in the drug discovery process.

TABLE 1 Examples of AI tools used in drug discovery

Tools	Details	Refs
DeepChem	MLP model that uses a python-based AI system to find a suitable candidate for drug discovery	[16]
DeepTox	Software that predicts the toxicity of a total of 12 000 drugs	[17]

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DeepNeuralNetQSAR	Python-based system driven by computational tools that aid detection of the molecular activity of compounds	[18]
ORGANIC	A molecular generation tool that helps to create molecules with desired properties	[19]
PotentialNet	Uses NNs to predict the binding affinity of ligands	[20]

4. DESIGNING METHODOLOGY

4.1 AI in designing drug molecules

Protein structure prediction based on target sequence It is crucial to identify the right target during medication development to provide effective treatment. Multiple proteins contribute to the disease and are sometimes overexpressed. Therefore, it is critical to predict the structure of the target protein to create the therapeutic molecule, allowing for specific disease targeting. Using the chemical environment of the target protein location, artificial intelligence (AI) can predict the 3D protein structure and so contribute to structure-based drug discovery [21]. Thus, researchers can foresee not just the effect a molecule would have on the target, but also any potential safety problems before the compound is even synthesized or produced. 25 out of 43 3D target protein structures were correctly predicted by the DNN-based artificial intelligence tool AlphaFold by analyzing the distance between neighboring amino acids and the matching angles of the peptide bonds.

AlQurashi employed RNN to make predictions about protein structures in his research. The author considered a recurring geometric network over three stages (computing, designing, and assessing) (RGN). A new backbone was created by taking into account the protein's basic sequence, the residue's torsional angles, and the intermediate backbone that had been built from the geometric unit. The last component produced the 3D model as its final product. Root mean square deviation (dRMSD) was used to evaluate the dissimilarity between the theoretical and experimental structures. When comparing predicted and experimental structures, dRMSD was kept small by optimizing RGN settings [22].

4.2 Predicting drug-protein interactions

The effectiveness of a treatment depends greatly on drug-protein interactions. Medicine repurposing and the avoidance of polypharmacy are both made possible through the ability to forecast how a drug will interact with a receptor or protein [21]. Better treatment efficacy can be guaranteed through precise prediction of ligand-protein interactions using various AI approaches. A support vector machine (SVM) model trained on 15,000 protein-ligand interactions based on original protein sequences and structural features of small molecules was utilized by Wang et al. [23] to identify new compounds that interact with four critical targets.

By combining pharmacological and chemical data, Yu et al. employed two RF models to predict potential drug-protein interactions; they then compared their results to those from established platforms like SVM, finding that their method was very sensitive and specific. Furthermore, these models predicted drug-target interactions, which can be

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expanded to target-disease and target-target connections to speed up the drug development process [24].

To collect reliable information from which to build iDrugTarget, Xiao et al. used the Synthetic Minority Over-Sampling Technique in conjunction with the Neighborhood Cleaning Rule. G-protein-coupled receptor (GPCR), ion channel, enzyme, and nuclear receptor (NR) drug-receptor interaction prediction is accomplished by a four-part subpredictor system (iDrug-GPCR, iDrug-Chl, iDrug-Enz, and iDrugNR). Through target-jackknife tests, this predictor was found to be more accurate and consistent in its predictions than previously used predictors [25].

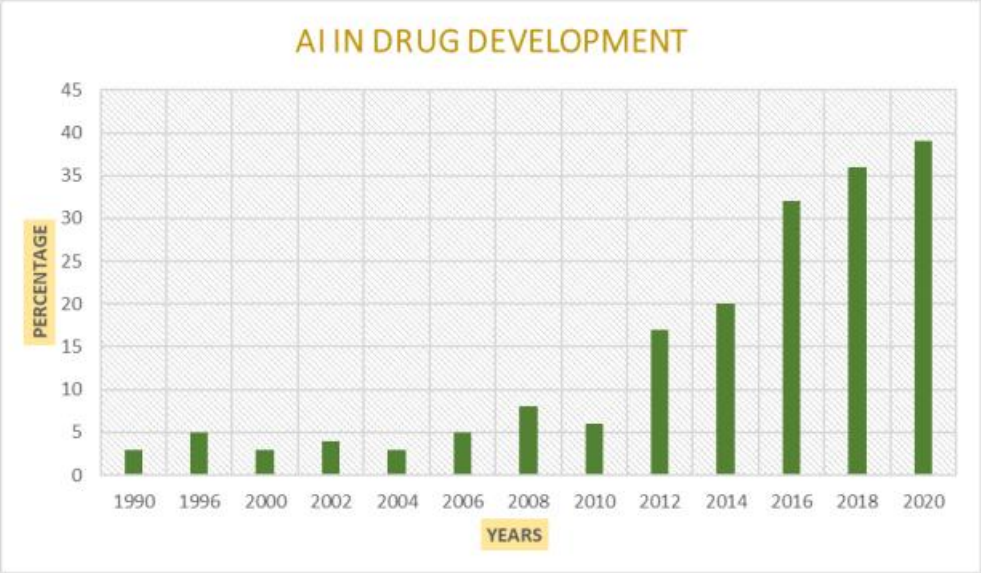

Figure 3: AI in drug development

4.3 Rethinking of drug design:

Despite advances in disease biology and considerable technology advances, the process of bringing new drugs to market is still lengthy and costly because of the high rate of clinical trial failures. [26] Several issues, which may be summed up as five "great challenges," need to be resolved for AI-assisted drug design to be effective in the long run. Producing and collecting relevant data, creating novel hypotheses, multi-objective optimization, lowering cycle times, and altering the research culture and mindset are all on the agenda.

4.4 Prediction of bioactivity:

To determine the drug's binding affinity, AI-based methods analyze shared characteristics between the drug and its target. The chemical moieties of both the medication and the target are utilized to establish the feature vectors for feature-based interactions. A similarity-based interaction, on the other hand, is predicated on the idea that drugs sharing structural or functional similarities with their targets will interact with those molecules. Predicting the therapeutic efficacy of medications and target proteins of known and unknown pharmaceuticals using unsupervised machine learning algorithms, such as MANTRA and Forecast, could help with drug repurposing and understanding the molecular mechanism of therapy.

4.5 Prediction oftoxicity:

The goal of "Toxicity Testing in the Twenty-First Century" is to develop better tools for predicting the potential risks that chemicals pose to human health. The atoms and bonds were depicted as nodes and edges in

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undirected, labeled graphs within the SDF format. To generate useful features, Deep Learning requires a large amount of training data. Successful models were labeled as "active," "inactive," or "inconclusive/not tested" based on the outcomes of the tests. In the past few years, high-throughput toxicity testing has generated a mountain of data that has made deep learning a viable option for toxicity prediction. [27]

4.6 Representation of ai in drug development:

Due to the high attrition rate and extensive planning required, bringing a new pharmaceutical to market can take several years and a substantial investment. Therefore, it is crucial to optimize this procedure using state-of-the-art tools, such as artificial intelligence (AI) (Figure 3). Recently, the FDA has been advocating for the use of RWD in the development of new pharmaceuticals. [28] Electronic health records (EHRs), administrative claims, and billing data are all examples of the kind of data that fall under the umbrella of "Research-Wide Data" (RWD) [29]. Only a small number of studies have used AI on RWD at different points in the drug development process; most of these applications have occurred in either the clinical or post-marketing phases. There were primarily three types of research that used AI on RWD: those aimed at optimizing trial recruitment, identifying adverse events, and repurposing medications. It has been estimated that between 68% and 39% of the pharmaceutical industry currently makes use of AI.

4.7 Limitations:

Artificial intelligence (AI) models are trained with data sets. Therefore, if the training dataset is inadequate, biased, or unequally distributed, the AI model's performance will deteriorate and its task outputs will be prone to errors. Developers of AI should work with medical professionals, ethicists, and philosophers to find solutions to problems that arise when applying ethical concepts to AI. [30] Rules should be drafted in this area to rein this in. Several obstacles arise when an AI attempts to use social media safety data, including but not limited to: misspellings, non-medical terms and slang, duplicates due to multiple postings, incomplete data due to missing important information, a lack of standards, a large volume of data, and a high signal-to-noise ratio (only a small proportion of drug safety data collected from social media contains information associated with ADRs).

CONCLUSION

There is a vast potential for the use of artificial intelligence. The most popular AI algorithms, such as deep learning-based algorithms, have their origins in the study of computer vision, NLP, and ASR. This context, however, makes it difficult to apply sophisticated AI methods to the task of developing new medicines. One, there is a great deal of complexity and a wide range of expertise required in the drug discovery process (biology, chemistry, and medicine; among others.). The drug development process, which has far-reaching consequences for public health and the pharmaceutical industry's bottom line, necessitates persuasive evidence for decision-making but is often overlooked. Despite this, numerous researchers have demonstrated the evident promise of AI technology in drug discovery in the future, and their significant efforts are discussed in this study. Even still, the gap between the two fields remains a significant obstacle. For this reason, 'drugdiscovery-specific AI technology can only be developed through close collaboration between AI professionals and other domain experts if the current state of drug discovery is to evolve. Experts in artificial intelligence will need to familiarise themselves with the

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specifics of drug development data to craft useful and interpretable algorithms capable of describing the modes of action and, thus, providing evidence for future decision-making. Additional domain experts will be required to generate low-error experimental biological and chemical data and store it in unified platforms if AI systems are to make any further progress. But the most important thing for both is a willingness to work together and communicate to create a real-world plan for a new revolution in medication development. To that end, we hope this review might serve as a useful springboard for filling in the blanks.

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