International Journal of Pharmaceutical Research and Applications
Volume 8, Issue 6 Nov-Dec 2023, pp: 1613-1620 www.ijprajournal.com ISSN: 2249-7781

Artificial Intelligence: Pharma Revolution

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Submitted: 25-11-2023 Accepted: 05-12-2023

ABSTRACT
Over earlier times ten years, drug discovery has seen a transformation because of artificial intelligence (AI). Several drug discovery applications, which includes virtual screening and drug design, have adopted the use of various AI techniques. In this article we first discuss about Artificial intelligence and drug discovery and it's related some applications. We also have mentioned AI based discovery and collaboration between AI companies and pharmaceutical companies. Typically, pharmacists strictly adhere to a rule-based process when discovering new drugs. But a new trend in research and practice is using artificial intelligence to drug development, either to enhance productivity or develop new medications for diseases that weren't previously treatable ailments. The process to discover new drugs could be completely transformed by artificial intelligence (AI), which offers increased speed, accuracy, and efficiency. Nevertheless, the effective use of AI relies on the accessibility of high-quality data, the resolution of ethical issues, and the acknowledging the shortcomings of AI-based methods. Overall, this review demonstrates the potential of artificial intelligence (AI) in drug discovery and brings light on the obstacles and possibilities facing this field as it attempts to realize its full potential and global scenario of Artificial intelligence in pharma revolution.

Keywords: AI, drug discovery, AI-based pharma companies, global scenario, challenges, application.

I. INTRODUCTION

Drug discovery is probably known as big-budget, complex time consuming process and have low success rates[1]. Drug discovery process is time consuming process and it's paradigms were faces various changes and developments in past centuries. Drug discovery is basically carried out by pharmacists. Disease can be defined as condition that badly affects to an organism and it's various functions along with humans. In this scenario, drugs or new drugs and medicine help to fight against diseases and this is the aim i.e. as old as human civilization itself [2].

"Artificial intelligence" the term was discovered by John MeCarthyin 1956 [3]. The use of artificial intelligence in medical science from past few years gives revolution to the pharmaceutical industry. Drug discovery is a process of developing or discovering and identifying new drug or medicine [4]. Day by day artificial intelligence enhancing their use. Scientists and doctors are involving in the development of this technology in medical and pharmaceutical industry. Recently artificial intelligence is use in pharmaceutical industry in four ways likely it is used to preventing complications during the treatment of disease, for the prediction of treatment whether it will be a successful or not for the patients. Used of technologies during operating the patients and the last one is to determine reason behind use of instruments and find new uses of that instruments to secure the safety and efficacy [5].

Drug Discovery in presence of AI

Drug discovery can be defined as the process of identifying the role of compounds which are bioactive for the development of new drug. New drug development process still facing many problem and challenges [6]. Now a days, Artificial intelligence has largely occupied drug discovery system. Artificial intelligence can be applicable for drug discovery in various stages [1]. Drug discovery process passed from trial-and-error method to the development of synthetic drugs [2]. One of the AI technique like 'machine learning' (ML) and natural language processing has potential to amend drug discovery process by using huge amount of data. By using deep learning (DL) it's become more easy to find the efficacy of drug compounds. Artificial intelligence can also predict toxicity of drug compounds [4] due to the digitalization of available data in pharmaceutical industry AIcan easily deal with this information in drug discovery. The drug discovery process is divided in four parts as follows drug design,

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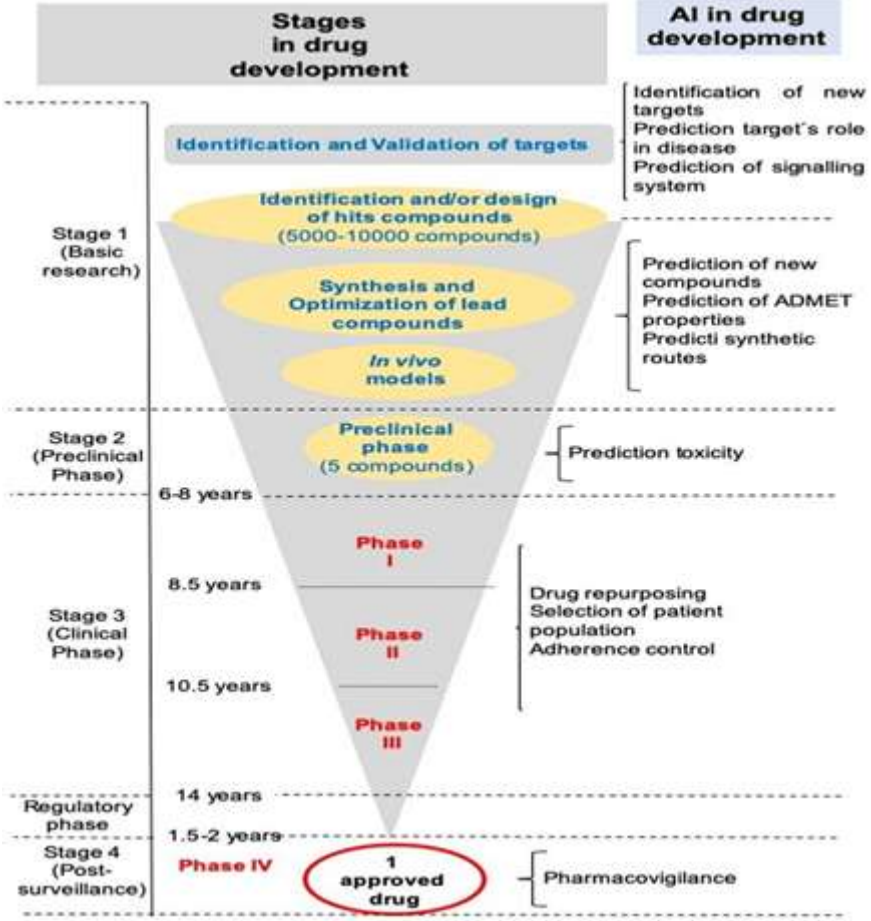
polypharmacology, drug repurposing and drug screening. Probably, AI is use to investigate the properties of drug, due to this reduce the need for clinical trials which also reduce the financial cost [5].Drug discovery involved into various stages. ML is a tool which is ligand binding target protein identified which is based on 3-D structure with DeepMind's AlphaFold which described 3-D protein structure by amine acid sequence QSAR is an example- QSAR means quantitativestructure-activity relationship is one kind of SAR. QSAR is integral part of drug discovery [8].

The Significance of Cooperation between Medical Professionals and AI Researchers

The development of novel and potent medicines for a variety of illnesses depends heavily on the cooperation of medical professionals and AI researchers.Combining their skills and experience allows them to develop potent algorithms and machine learning algorithms used to forecast possible treatment candidates' efficacy help expedite the process of finding new drugs. Additionally, this cooperation may enhance the precision and effectiveness of clinical studies, since data analysis can be done using AI algorithms gathered throughout these trials to spot patterns and any possible side effects of the medications being put to the test. This can assist pharmaceutical businesses in making well-informed choices regarding select medication candidates to investigate and can expedite the entire drug [9][10].Given that AI can support intelligent drug development, aid in decision-making, and be involved in the development of a pharmaceutical product from the bench to the bedside, it is conceivable that AI would be used in this process. Choose the appropriate course of treatment for a patient, including customized medications; as well as oversee and utilize the clinical data produced for upcoming medication research [11][12].

Stages involved in AI drug discovery

Fig. 1: shows that graphic process diagram that shows the stages involved in creating pharmacological active molecule with comparison of stages in drug discovery and AI in drug development.



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Sr. No.	Company	Year	Country	Major Application	Revenue	Link
1	Biovista	1996	USA	Drug re-positioning, derisking and personalized medicine	4M USD	https://www.biovista.com/
2	Valohealth	2007	USA	Integrated system for end-to-end drug development	19.4M USD	https://www.valohealth.com//
3	Verge Genomics	2015	USA	Drug discovery for neurodegenerative treatment	2.78M USA	https://www.vergegenomics.com/
4	Insilico medicine	2014	Hong Kong	AI-based identification of drugs	10.9M USA	https://insilico.com/
5	iCarbonX	2015	China	Multi-omics technologies for innovative biomarkers	5M USA	https://www.icarbonx.com/en/
6	Trials.ai	2016	USA	Intelligent AI clinical design	1.2M USA	https://www.trials.ai/about
7	ReviveMed	2016	USA	AI-based drug design for metabolomic disease	0.26M USA	https://www.revivemed.io/
8	Nuleome Therapeutics	2019	UK	Decoding dark genome for new ways of disease	6.3M USA	https://nucleome.com/
9	Insitro	2018	USA	Predictive Models for Drug design	20.6M USA	https://insitro.com/
10	PathAI	2016	USA	Digital pathology analysis for drug design	255M USA	https://www.pathai.com/
11	Deep Genomics	2014	Canada	AI-based platform for complexities in RNA biology for	9.5M USA	https://www.deepgenomics.com/

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				drug design		
12	Verantos		USA	Real world evidence company for Clinical, regulatory claims		https://verantos.com/
13	OneThree Biotech	2018	USA	AI-based drug design platform for multiple clinical validation	3.5M USA	https://onethree.bio/
14	Aria Pharmaceuticals	2015	USA	Small molecule development	5M USA	https://ariapharmaceuticals.com/

Table 1: List of AI-based pharmaceutical and biotechnology companies in the drug discovery

Fig. 2 : Shows the emergingstartups transforming healthcare with AI

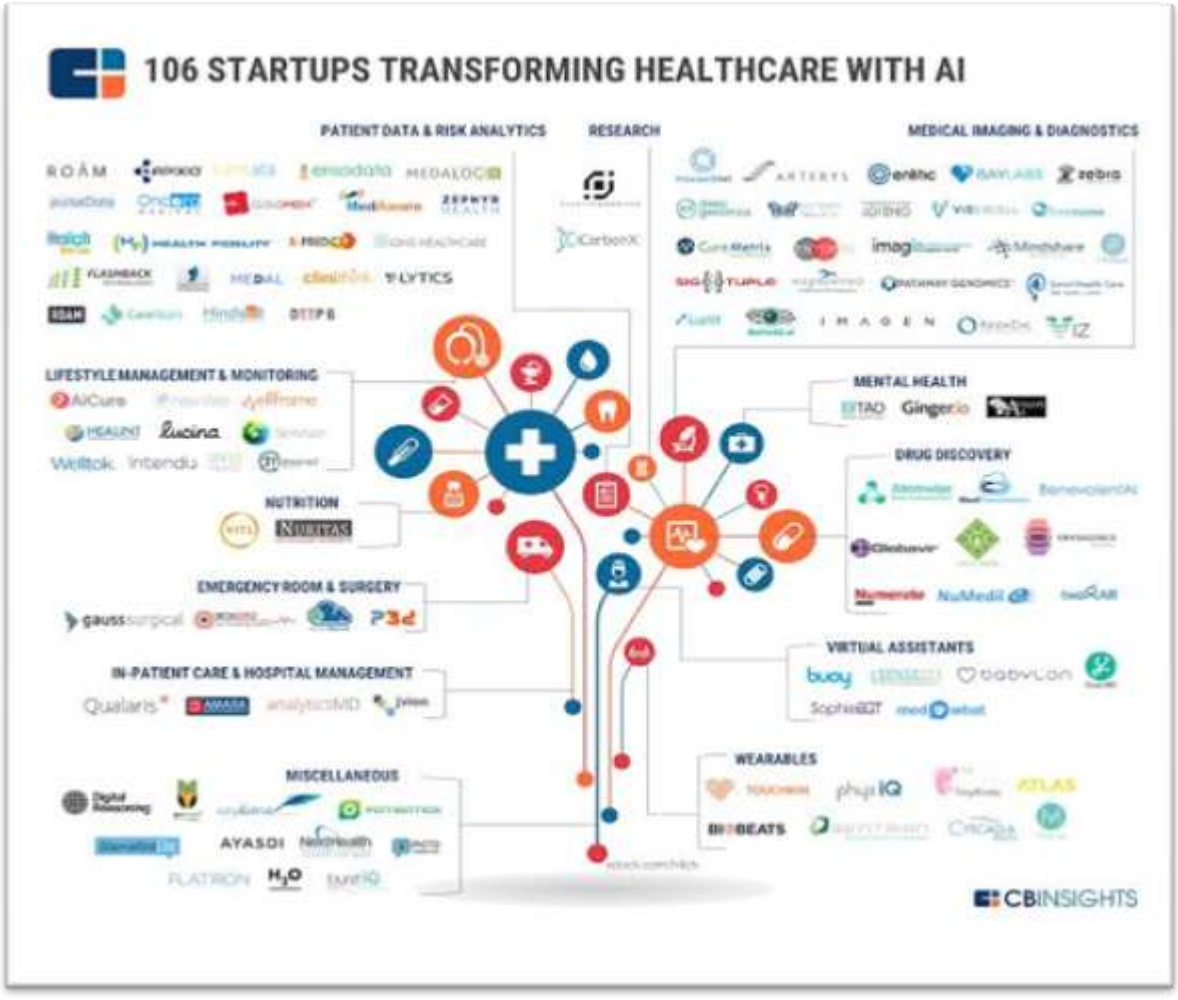

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Table 2: List of AI-based drugs

Name of Drug	Purpose	Company	Status	Reference
DSP-1181	Treatment of OCD	Exscientia in collaboration with sumitomo Dainippon Pharma	Entered phase-1 clinical trials on January 30,2020	13
EXS21546	Immuno-oncology drug	Exscientia in collaboration with Evotech	Entered phase-1 clinical trials on April 09, 2021	14
DSP-0038	To treat Alzheimer's disease psychosis	Exscientia in collaboration withsumitomo Dainippon Pharma	Entered first phase of clinical trials on May 13, 2021	15

Current status at global level

Artificial Intelligence (AI) is continuously growing in health care sector with greatest revolution in digital era. At global level artificial intelligence in drug discovery and development market is grown up from $1.04 billion in 2022 to $1.38 billion in 2023. The annual growth rate i.e compound annual growth rate (CAGR) is 31.9% [16]. In this digital era, artificial intelligence. Will change the medical field. Artificial intelligence is one of the best technology which is going to provide all life expectancy [17]. Year by year pharmaceutical companies are diverted to artificial intelligence (AI) companies to decrease the financial crises and to reduce the chances of failures in the discovery. Around 40%. Of growth during 2017 to 2024 triggers the global market which can show the extraordinary revolution in pharmaceutical and medical field []. There are huge chances to grow AI market in drug discovery up to $3.74 billion in 2027 at CAGR of 28.4% [18].

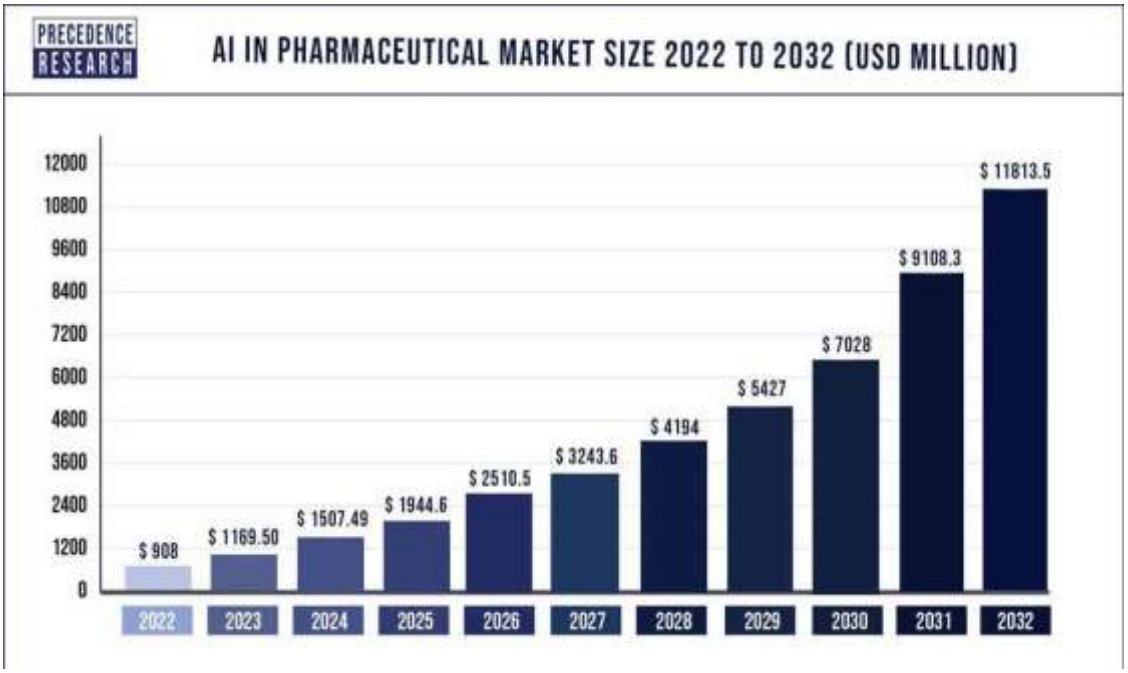

Fig. 3 AI in pharmaceutical market size since 2022 to 2023

Challenges

Notwithstanding AI's potential advantages in drug discovery but there are a number of obstacles and restrictions to take into account. Availability of suitable data is one the challenge facing in AI drug discovery[19]. A lot of data is usually needed for AI-based techniques in order to train them. Many times, there may be a limit to

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quality of data that is available, or the data may be inconsistent or of low quality, which may have an impact on it's accuracy and dependability [20][21]. Making sure AI is used fairly and ethically develop novel therapeutic compounds is crucial consideration that needs to be taken into account [22]. The knowledge and experience of human researchers cannot be replaced by current AI-based techniques, nor can they take the place of conventional experimental procedures. AI can only make predictions based on the data that is currently available, the finding them need to be verified and evaluated by researchers who are human [23][24][25].

Application

There is an evidence that AI application are beginning to proliferate in the drug discovery and design field [26].

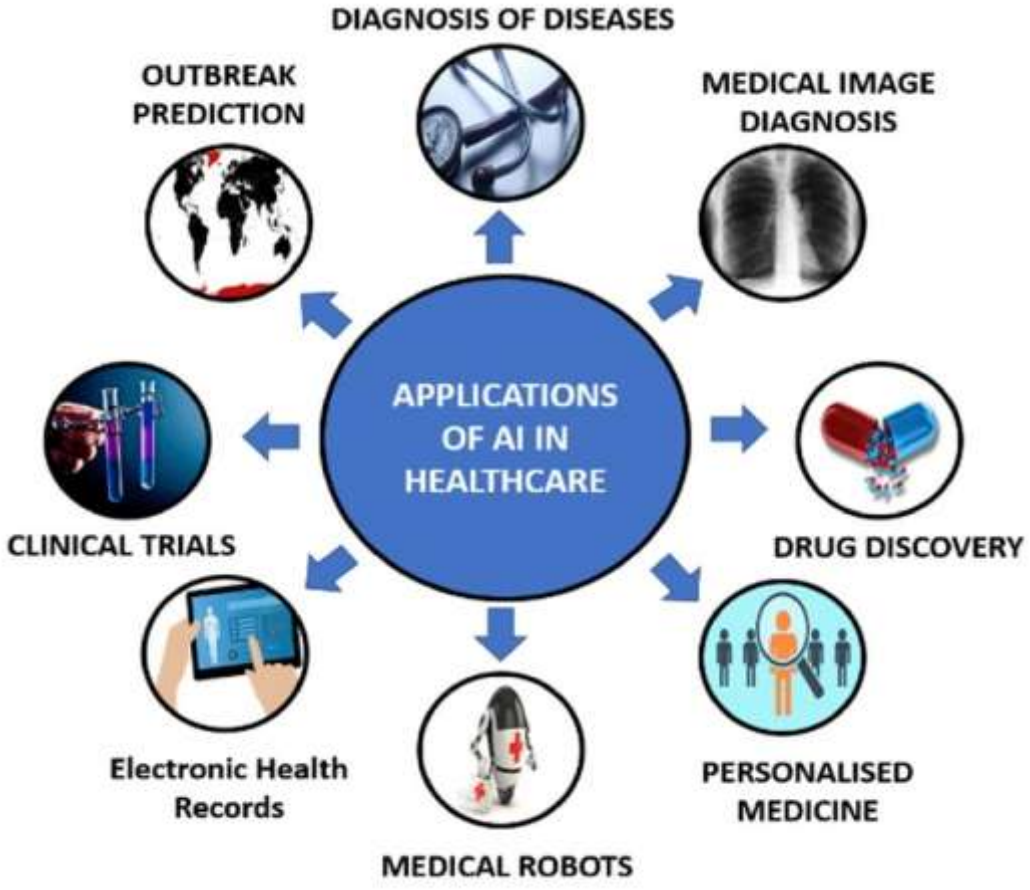

Fig. 4 Application of AI in healthcare

II. CONCLUSION

The health care industry is embracing AI-based techniques, which impact areas like drug design, diagnosis, prevention, and clinical recommendation making. These techniques are intelligent, flexible, and low-cost. Applications of AI were previously believed to be less effective than combinatorial chemistry, experimental high-throughput screening, and other technical forces. Using computer programs to create new chemical entities with the desired features from scratch was challenging.Possibly superior to a human specialistUsing data science techniques for target identification, De novo molecular design, drug repurposing, retrosynthesis and reactivity and bioactivity prediction, FDA approval, and post-market analysis can speed up the prolonged and expensive process of drug design. Some pharmaceutical companies have used AI, and the results have been revenue from AI-based pharmaceutical solutions, which are projected to generate US $2.199 billion by 2022. In order to

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increase prediction power when determining the characteristics of small molecules, deep neural networks (DNNs) can be utilized and in the absence of a substantial quantity of experimental data, one-shot learning can be employed. Having a technical and to produce meaningful models for prediction, human error, labelling restrictions, and biological variability related to the underlying data are essential models. AI merely provides a platform for plans to be carried out; great things arise in minds and are never achieved alone. We must use the expertise of various domain experts to create novel ideas for drug discovery. Next, we can create an algorithm for data analysis, and after that, we can adjust the algorithms or the hypothesis based on what we have learned from the data. Briefly put, both minds and machine must cooperate with one another. We anticipate seeing a rise in the application of machine learning in the future, particularly deep learning and aid in the development of semi-automated smart particles, help us comprehend intricate biological systems, and AI is also anticipated to speed up drug development, be a useful tool in the study of human biology, and act as a catalyst in the fight against human diseases. Quality and safety are more crucial for drug discovery than speed and cost, so it's very difficult to create an AI system that can achieve this multi-objective optimization in a multidimensional complex space which requires interdisciplinary cooperation in both academia and business.

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