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ROLE OF ARTIFICIAL INTELLIGENCE IN DRUG INDUSTRY

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ABSTRACT

The use of artificial intelligence (AI) in drug creation has pioneered a revolution in pharmaceutical research by incorporating powerful computational methods with traditional biomedical research to overcome longstanding challenges. This review describe the application of AI in drug design polypharmacology, chemical synthesis, drug repositioning and prediction of drug properties including toxicity and bioactivity and other physicochemical parameters. There are also prospects for development but rather details the problems which face the development of AI technologies in the field of including data quality generzability, computational power, and ethical issues.

INTRODUCTION

Drug discovery encompasses those efforts involving the biological assay that will result in the creation of drugs designed to improve some aspect of human health by preventing or including diseases. This process, which is very critical for the realization of effictive drugs in the medical field, involves various steps starting from identification of a target, lead discovery, hit to lead, lead optimization, preclinical evaluation and clinical evaluation. Historically the need of this process was considered and interciate as it has been estimated That it takes an average 12 years and costs 2.6 billion to advance a single molecule from invention to the FDA approval process. This phenomenon, has been accomptained by

high attrition, signification side effects associated with modern medicines, and inability to manage chronic illness like diabetic and cancer more effectively.[1,2]

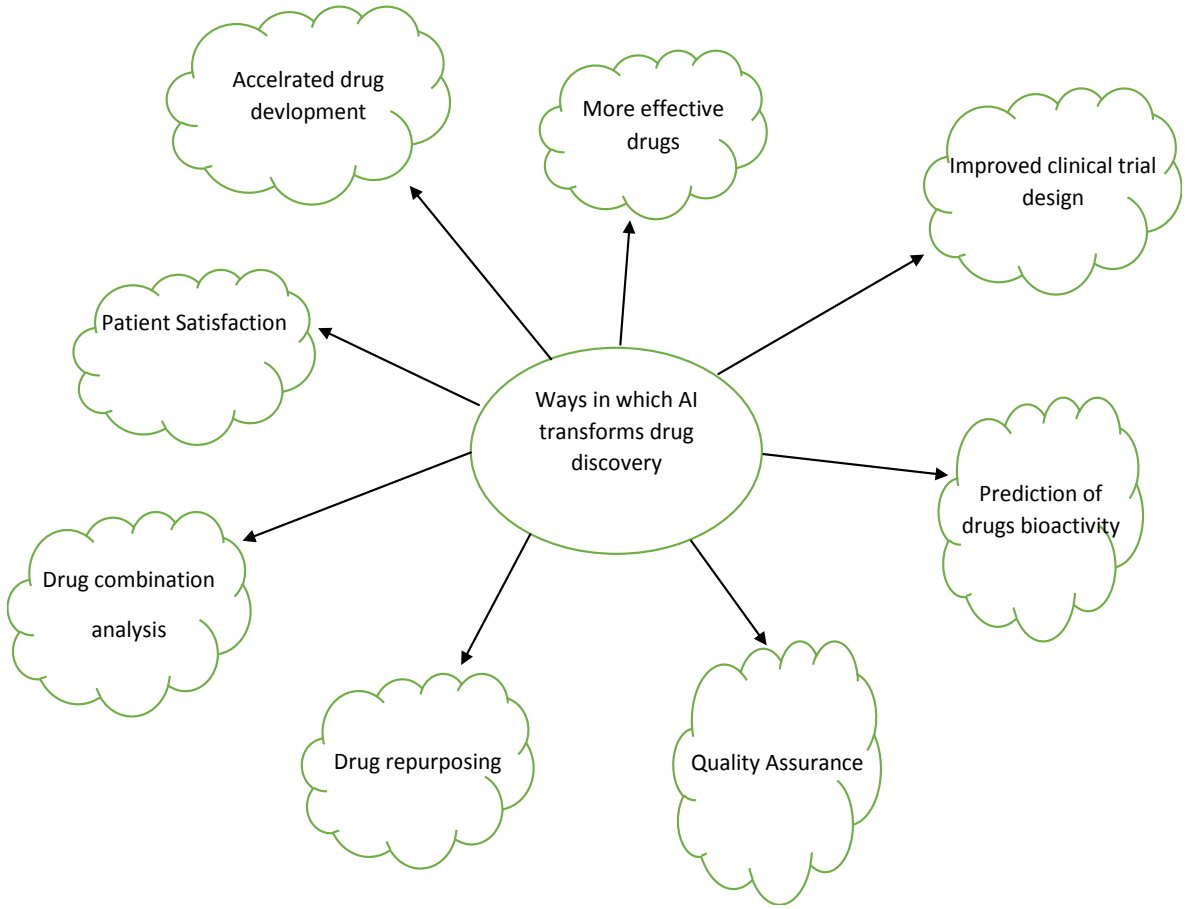

Fig. 1.

Benefits of AI in drug discovery

1. **Accelerated drug development**

- Artificial intelligence accelerated drug development by replying on data driven insights. Predictive modeling can help AI quickly identifying potential drug candidates and potential interaction without extensive lab work, High throughout screening in enhance as AI sifts through massive chemical libraries to pinpoint effective compounds. It also assists in designing drugs by proposing new chemical compounds or optimizing existing ones thereby minimizing the cycle of trial and error. AI is also fastening up clinical trials by selecting ideal participants for the study so that more efficient and speedy trials can be conducted generally, AI reduces the timeline from discovery to the approval of drugs and develops new drug much faster.[10]

2. Prediction of drugs bioactivity

- Drug discovery is one of the many fields where AI can be applied for instance, predictive modeling is also based on its use by using AI technology.[3]
- It can analyze vast amounts of biochemical data to identify patterns, recognize potential bioactive compounds, and ultimately assists researchers in a more efficient way to identifying promising pharmaceuticals.[12]
- AI employees several methods such as machine learning (ML) deep learning (DL) and natural language processing (NLP) that analysis of biochemical data and allow to predict bioactivity. Therefore these techniques can be used by AI for learning from bigger datasets and providing precise forecasts on the bioactivity of potential drug compounds.

3. More effective drugs

- The significance of AI in drug discovery and development is crucial as it helps in predicting the pharmacological properties of lead molecules according to their chemical structure thus making bringing forth an efficient process for drug development. Employing machine learning algorithms, researches could come up with predictive models for key properties such as solubility, bioavailability, and toxicity .The new molecules designed from such models have better pharmacological characteristics than those earlier developed targeting a more effective and soft therapy.

4. Improved clinical trial design

- The clinical trial design is revolution due to the inclusion of AI through patient selection improvement, medicine personalization and real time trial parameter adaptation. Machine learning and natural language processing among other AI technologies help optimize trial efficiency, precision and patient results.[16]
- Data management is made smoother by AI in addition to identifying new biomarkers by AI in addition to identifying new biomarkers and best dosing strategies, Along with regulatory compiles by AI, virtual trials enhance availability.[11]
- Pfizer, IBM Watson, and oracle health science leverage AI for clinical trial innovation.

5. Quality assurance

- It is through automating examinations foreseeing problems and guaranteeing conformity that artificial intelligence spur on quality assurance revolutionarily, Enhancing precision, productivity and client satisfaction are some of the impact of technology such as machine learning as well as natural language processing in AI. The application of AI centered QA

spans across different industries including software engineering, manufacturing process control, healthcare system management and finance among others using application like Test complete, selenium or JIRA among other with the introduction of AI into QA department within organization they achieve reduced defects rates.

- Along sides lesser expense and postponements on production cycle while enhancing overall quality.[10]

6. Drug repurposing

- Artificial intelligence is developed to accelerate drug repurposing through new indication of existing drugs analyzing large data and predict efficacy and safety AI in ancology, neurology, infection disease and rare disease processing (NLP). AI reducing the development cost and time increasing efficacy and safety different database used for drug repurposing are Drugbank[6], Pubchem, Deepchem, etc. In future, multiomics data will be used and develop explaination model.

7. Drug combination Analysis

- Artificial intelligence improves drug combination analysis by making prediction of synergistic analysis, by making prediction of synergistic effect
- Revealing new interaction and reducing experimental space in the clinic. AI technology can explore and analyze large scale data to find effective drug combination for disease like cancer machine learning, deep learning and network analysis based AI can do-
- Predict drug – Drug interaction
- Identify optimal dosage regimens
- Prioritize combination for clinical testing[17]
- AI driven platforms like Deepchem, Atomwise and chemBL fast tracking drug combination.
- AI is saving in trial costs and helping improve the efficiency of such combination and enhance patient outcome by developing personalized combination therapies for aliments like cancer, HIV or TB.[14]

8. Patient satisfaction

- Artificial intelligence helps in personalizing patients care plan, efficient communication and accurate diagnose. AI chatbots and predictive analysis provide 24/7 availability, instant response and health specific information access to the patients that increase the

patients involvement, satisfaction and healthy behaviour of the patient while decreasing re-admission rate. AI based service platforms analyze an huge amount of data generated from patient, treatment patterns and get insights of their patient preferences worries issues that results better compossioned and humanist approach for ensuring best customized core to the patient. Overall, quality efficiency improvement and satisfied patient can be achieved using AI.

Application of AI in drug discovery

1. Target identification

Taking a step towards better target identification for instance in drug discovery, artificial intelligence, has become able to correlate genomic and proteomic data, produce structural and functional prediction of proteins, as well as determine possible binding site technology such as machine learning and deep learning help minimize the occurance of inaccurate observation and improves the comprehension of the underlying mechanism of the ailment.[15] Studies include cancer, diabetes affecting the brain, the spread of disease, and the units by which the population is divided – the disease of the few natural users interfare including Deepchem, Atomwise, chemBL, etc. Help in to researches to validate the proposed drug targets by employing the analytical power of the AI to increase the chances of finding a safe and effective drug.

2. Gene- disease association discovery-

- Gene-disease association can be researched using AI by examining genomic information trends, and establishing correlations to locate genes that are links to disease, AI employees genomic data sequencing, gene expression data, and mining literature.[15] Several features that ensure that expansion and prediction of new relationships for on implementation of `1personolized medicine. AI increase precision minimize the incidence of false alarms, and significantly fastens the process of understanding complete disease such as cancer and other neurodegenerative disorder. This leads to
- To development of more effective treatment regimens and improvements in patients prognosis.

3. Predicting drug-drug interaction and toxicity

- Using an AI it can very precisely forecast drug safety properties in terms of drug-drug interaction or drug toxicity. This is due to the ability of AI algorithms to predict such molecules changes, structural alteration, measures toxicity and analyze generic

information like clinical and pharmacological profiles of other drugs for instance, Deepcham, and Atomwise use machine learning and deep learning AI, where adverse events interaction amongst drugs and toxicity are predicted using chemical structural transformation of target molecules. This reduces the rate of adverse events, enhance the efficiency of drug development process and promotes patient safety by enabling use of precision medicine.[8]

4. Precision medicine

- The field of precision medicine is largely enhance through AI which makes it possible to integrate genomic, phenotypic and clinical data for the purpose of exploring treatment option. Machine learning and deep learning are examples of AI application that assess risk and allow appropriate intervention to disease progression. Uses include cancer treatment heart disease management of rare genetic syndrome advanced computer platforms for intance, Deepchem, and IBM watson for genomic is addition to improving the efficiency of treatment reduce adverse reactions of the patient and hence improving clinical outcomes.[14,11]

5. De-novo drug design

- AI changes the paradigm of the de novo drug design through innovation structure generation efficacy, and safety prediction lead optimization and target identification. Technique development within AI such as machine learning deep learning and generation models allow for a rapid and effective design pipeline advantages of this changes are higher efficiency lower cost higher quality, improved safety, and speeded up drug discovery. Use case is not limited to cancer or brain disease, but also includes com addresses infections disease and even includes complex rare genetic disorders.[4,5,7]

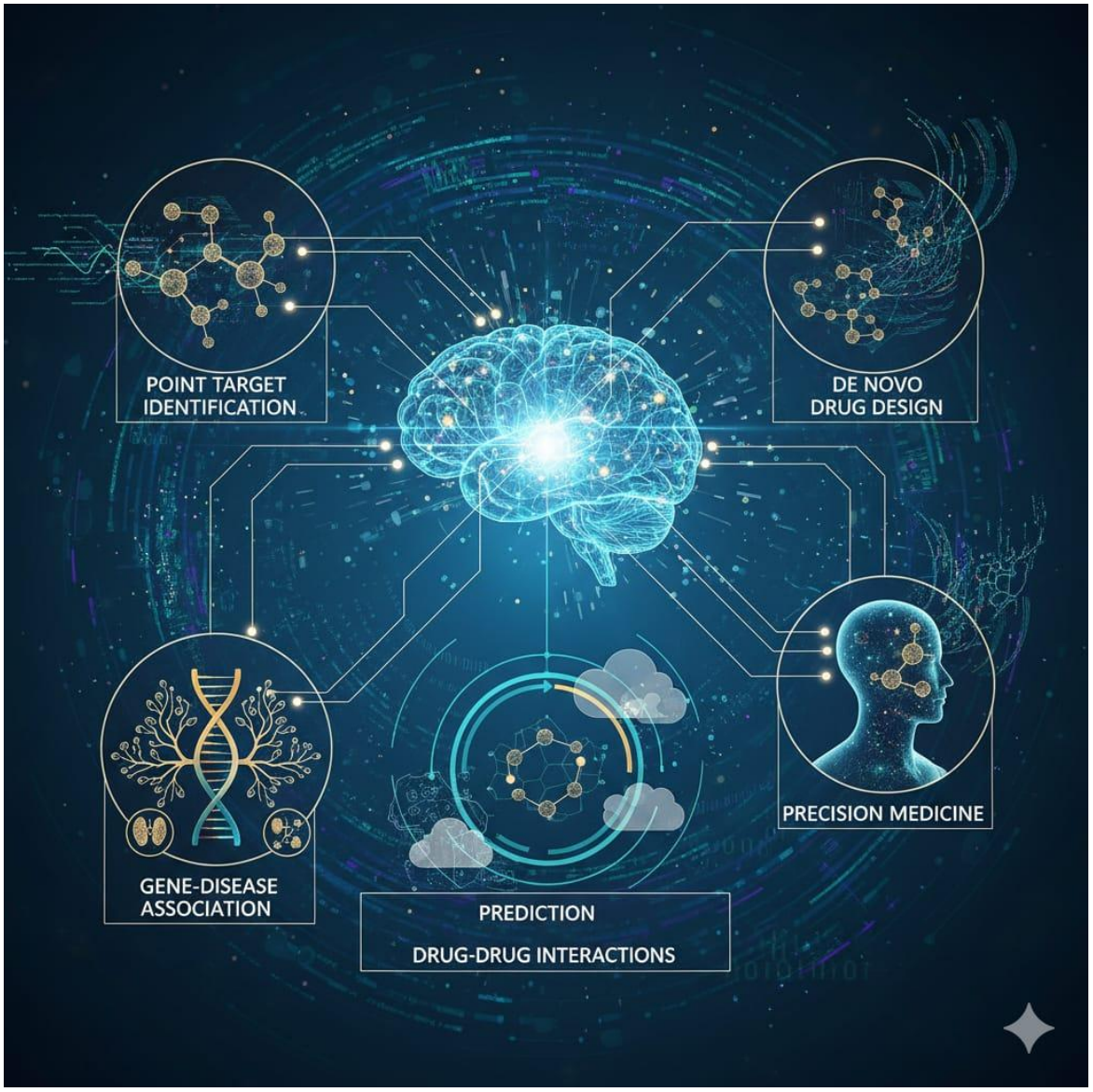

Fig. 2.

Real world AI drug discovery examples

1. Insilico medicine

- Insilico medicine is pioneer in AI driven drug discovery.
- In 2001, the company successfully used its AI platform to identify a novel drug target and design a new small molecules drug for idiopathic pulmonary fibrosis.[4]

2. Exsecientia

- Exsecientia is UK based company that uses AI to design drug faster than traditional methods. In 2020, Exscientia in collaboration with sumitomo Dainippon pharma, become first company to bring on AI designed drug to

- To clinical trials. The drug DSP-1181, is designed to treat obsessive-compulsive disorder.[9]

3. Benevolent AI

- Benevolent AI uses AI to analyze vast amount of biomedical data scientific literature to identify new drug targets and treatments one of its significant successes was identification of BARICITINIB as a potential treatment for COVID-19.

Challenges of using AI in drug discovery

1. Issues faced while utilizing AI for drug research

- A. Quality and availability of information[13]
- B. fusing varying types of information
- C. Harmonizing data types
- D. Dealing with many variables.

2. Issues regarding algorithms

- A. AI model comprhession
- B. Eliminating prejudice from training set
- C. Optimal algorithm selection.

3. Legal challenges

- A. The legal environment of discovery with use of AI tool
- B. Evaluation of AI outputs
- C. Copyright

4. Research challenges

- A. Comprehension of biological system with many components.
- B. Predicting the interaction of protein with a ligand.
- C. Considering absorption – distribution – metabolism – excretion of drugs.[19]

Fig. 3.

- **Future of AI in drug discovery**
- AI in drug discovery has excellent future potential. In the immediate near term that is between 2025 and 2030, it will see an integration of workflow with experimental validation and considerable machine learning and deep learning being scattered across the workflows, Between 2030 and 2040, de-novo design will begin to take shape as possible with generation models, multi-omics data integration will advance, and synthesis followed by AI driven testing in a workflow will become common, personalized medicine will take off.
- Looking forward to 2040-2050, AGI will revolutionize drug discovery, enabling fully automated design and testing of drugs, predictive models for complex disease and a shift

in the industry itself. Some of the emerging trends include Explainable AI (XAI) transfer learning quantum computing and blockchain for data security.[18]

- Data quality, regulation framework, AI interpretability and managing the expectation of stakeholders remains to be same of the challenges. However these not with standing, AI holds a great promise for drug development; drugs developed much faster by 50-70% more often than with traditional approaches, cheaper, reduced costs 30-50%; personalized treatment for complex diseases, wit time, AI will transform the pharmaceutical industry.[5]

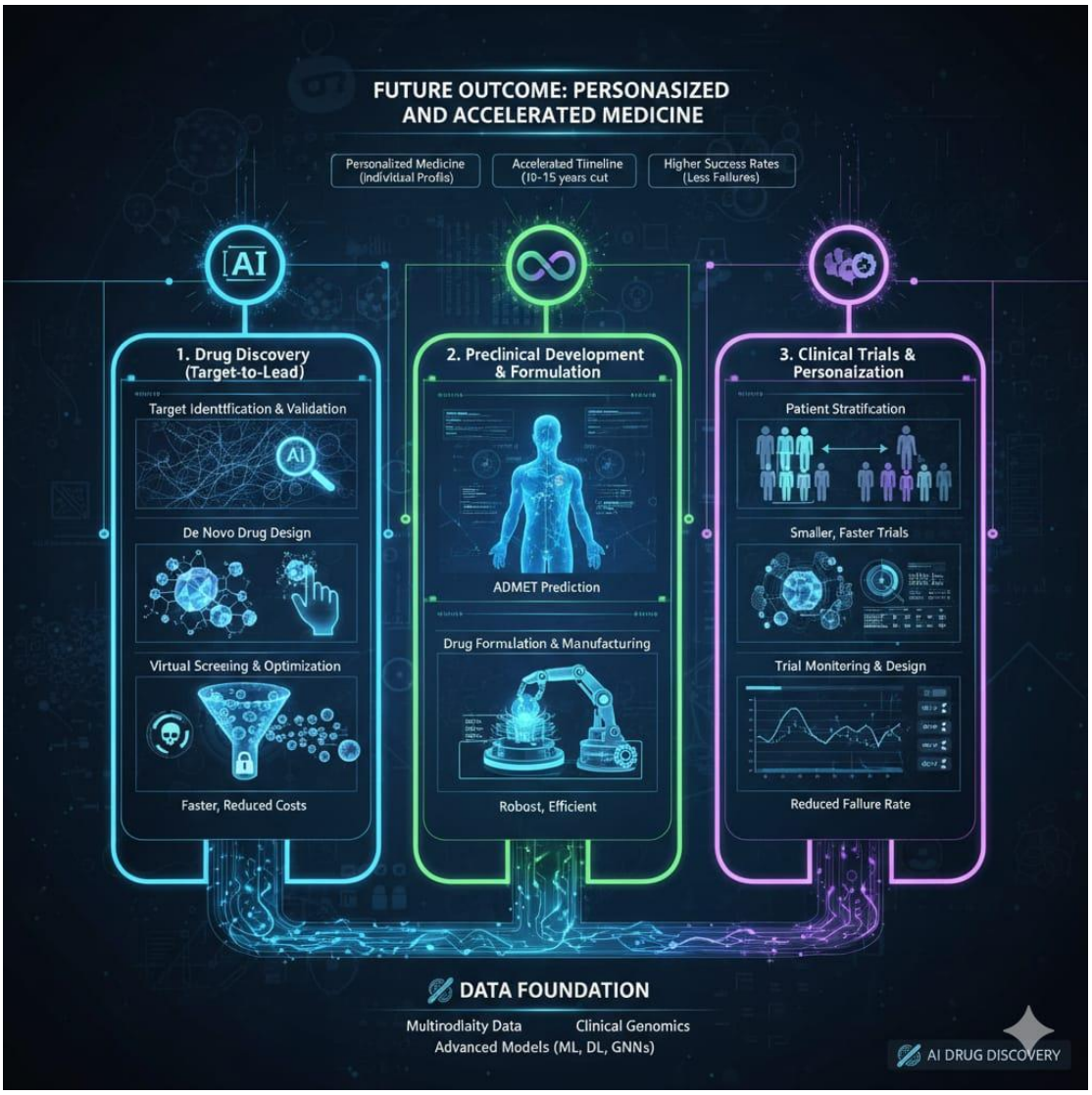

Fig. 4.

CONCLUSION

- The integration or rather the combination of AI drug discovery has the ability to change the pharmaceutical and healthcare delivery system in a very big way. For instance, it can shorten the time taken in drug development, improve the design of clinical trials, Forecast

the in-vivo activity of drugs and do quality assurance. As a leading edge and very innovative AI development company, provide quicker, cheaper and more

- Effective solution that are responsible for development in the medical field and other life saving therapies.[20]

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