AI USED AS A TOOL IN DRUG DISCOVERY AND DEVELOPMENT:

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ABSTRACT

Artificial intelligence (AI) has appeared as a transformative tool in modern drug development and discovery. It uses advanced algorithms and machine learning (ML) techniques to analyze large biological and chemical dataset quickly and accurately. This opinion review critically examined the feasibility and prospects of integrating AI as a tool in the pharmaceutical industries. This opinion review delved into the current landscape of AI driven approaches, discussing their utilization in target identification, lead optimization, and predictive modeling of pharmacokinetics and toxicity, thereby reducing experimental failure and casts. AI technologies-such as Machine learning (ML). Deep learning (DL), natural learning processing (NLP), and neural networks. AI assists researchers in identifying novel drug targets by analyzing vast biological dataset, including genomic, proteomic and metabolic information. It also supports virtual screening and structured based drug design, allowing scientist to predict molecular interactions and binding affinities before laboratory testing. Our in-depth comparative analysis highlights the advantages, limitations, and practical challenges associated with different AI approaches, emphasizing critical factors and successful implementation such as data quality, model validation and ethical considerations .AI future directions to unlock the full potential of AI in creating safer, more effective, and accessible medicines. By emphasizing transparent methodologies, robust validation, and ethical frameworks, this review aims to guide the responsible and impactful integration of AI into pharmaceutical research and development.

In clinical research, AI tools are used for biomarker discovery, patient satisfaction and clinical trial optimization, improving the efficiency and safety of new drug and enhance the productivity.

Overall, AI serves as a transformative tool that bridges the gap between computational science and pharmaceutical innovation. By integration AI with bioinformatics and cheminformatics, the future of drug discovery is expected to become faster, more cost effective, and more precise, ultimately leading to the development of safer and more effective therapeutic agent.

KEYWORDS

Artificial intelligence, Machine Learning, Deep Learning, Drug Discovery, Drug Development, Virtual Screening, Target Ingredient, Lead Optimization, Predictive Modeling, Molecule Docking, Structure Based Design, Biomarker discovery, Big Data Analysis, Computational Biology, Pharmacokinetics, Pharmacodynamics, Drug Repurposing, Precision medicine, Conclusion.

Introduction

Drug discovery and its development is very long, complex, and very expensive process which takes more than 10 years to complete whole process. Each stage, from identification of molecule to final approval for marketing carries high risk of failure, and very less drug applicant reaches to the market. This makes the process expensive and inefficient.

AI has the potential to revolutionize the drug discovery process, offering improved efficiency, accuracy, speed and also improving pharmaceutical productivity and clinical trials. AI reduces the human workload as well as achieving targets in a short period of time.

However, the successful application of AI is dependent on the availability of high-quality data, the addressing of ethical guidance and recognition of the limitation of AI – based approaches.

AI, mostly machine learning technique has also been carried out to evaluate toxicity. For example, the DeepTox platform is used to evaluate the toxicity in any compound and MoleculeNet, is used to determine molecular

structure and predict it's toxicity.

Various Pharmaceutical Companies have used AI to improve their drug drug discovery. Most neurological disease are polygenic, but companies data targets one gene. In 2018, Verge Genomics developed an algorithm for identification of pathogenic genes and select the drug to target them. In this process company utilities the vast potential power of AI technology.

Novartis currently uses AI technology to classify different cell's digital image. In this each cell is treated with different experimental molecules. To find biological active molecule it require very complicated analysis. Therefore for speed up the process the company used machine learning algorithms for predicting unknown molecules.

In this article, the benefits, challenges, and drawbacks of AI in this field are reviewed, and possible strategies and approaches for overcoming the present obstruction are proposed.

The purpose of this study was to discuss how artificial intelligent (AI) methods affect the field of drug development. Modern application of AI in nanomedicine design and pharmacological synergism or antagonism prediction were also covered.To fully realize the promise of AI in drug discovery, the review unknowledge the difficulties that come with its uses in this field and advocates for more study and development.

In summary, artificial intelligent and deep learning advancements provide on excellent opportunity for rational drug design and discovery process, which will eventually impact mankind.

The goal for this review were: To assess the current state of AI in drug discovery and development, To investigate how AI has impacted various stages of drug development, Too identify key challenges and limitations related to AI based drug discovery and to show case studies and success stories where AI based approaches has led the discovery of promising drug of existing for new indications and to provide insight to potential future directions and trends in AI based drug discovery and drug development.

Drug Discovery:

Historically, experiments were recorded in paper lab notebooks, and they collected for patent purpose. But in preceding 10 years, paper notebooks have been substituted by electric lab notebook to enhance privacy and for basic information registration, entry and recovery.Drug discovery and development are among the most important translational science activities that contribute the human health and wellbeing.The discovery and advances of medicines may be considered as the ultimate relevant translational science effort that adds to human indestructible secure and happiness. However, the development of a new drug is very complex, expensive and long process which typically costs 2.6 billion USD and takes 12 years on average.

PROCESS OF DRUG DISCOVERY:

The process of drug discovery is done in following major stages:

- Target Identification and Validation.
- Lead Compound Identification.
- Lead Optimization.
- Preclinical Testing.
- Clinical Trials.
- Regulatory review and post marketing.

1) **Target Identification and Validation:** Scientist and researchers identify specific molecule targets involved in disease. After that they confirm that acting of these target molecules could result in therapeutic effects.

2) **Lead Compound identification:** Scientists search large number of chemical libraries to find compound that can interact with the selected target disease. After that these compounds are refined into leads-compounds with improved potency and selectivity.

3) Lead optimization:

In this stage, lead compounds further undergo modification to improve and enhance their biological activity, selectivity, pharmacokinetics and its safety profile. The most suitable compounds are selected for advanced development.

4) Preclinical testing:

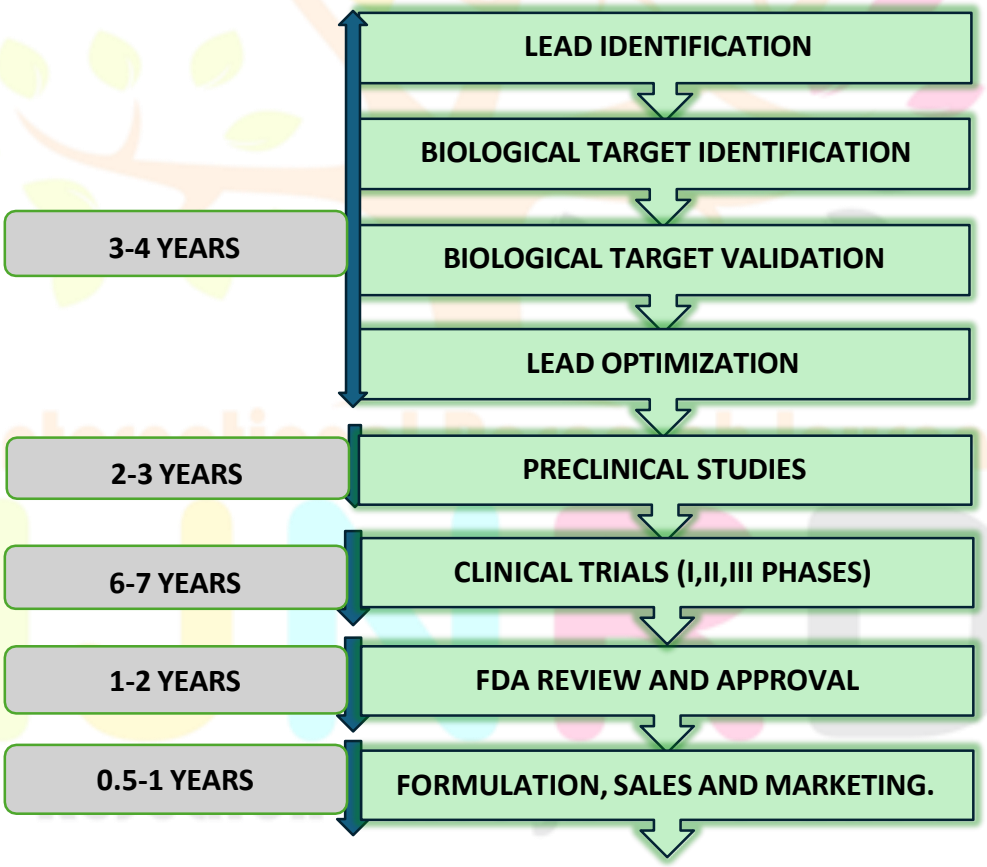
After identification and modification of lead compound, most potential compounds are tested in vitro (in the lab) and in vivo (in living models) to collect evidence of their safety, efficacy, and suitable dosing before human trials.

5) Clinical trials:

Clinical trials means testing of new formulated chemical drug in human body. The human testing starts in different phases (like: I,II,III) to check efficacy, safety and dosage. Only a small percentage of drug or compound pass these phases to enter in market.

6) Regulatory review and post-marketing:

It is the last stage in the process of drug discovery. After successful clinical trials, regulatory agencies review all data related to drug compound before approving the drug for public use. Post-marketing surveillance ensures ongoing safety in the population.

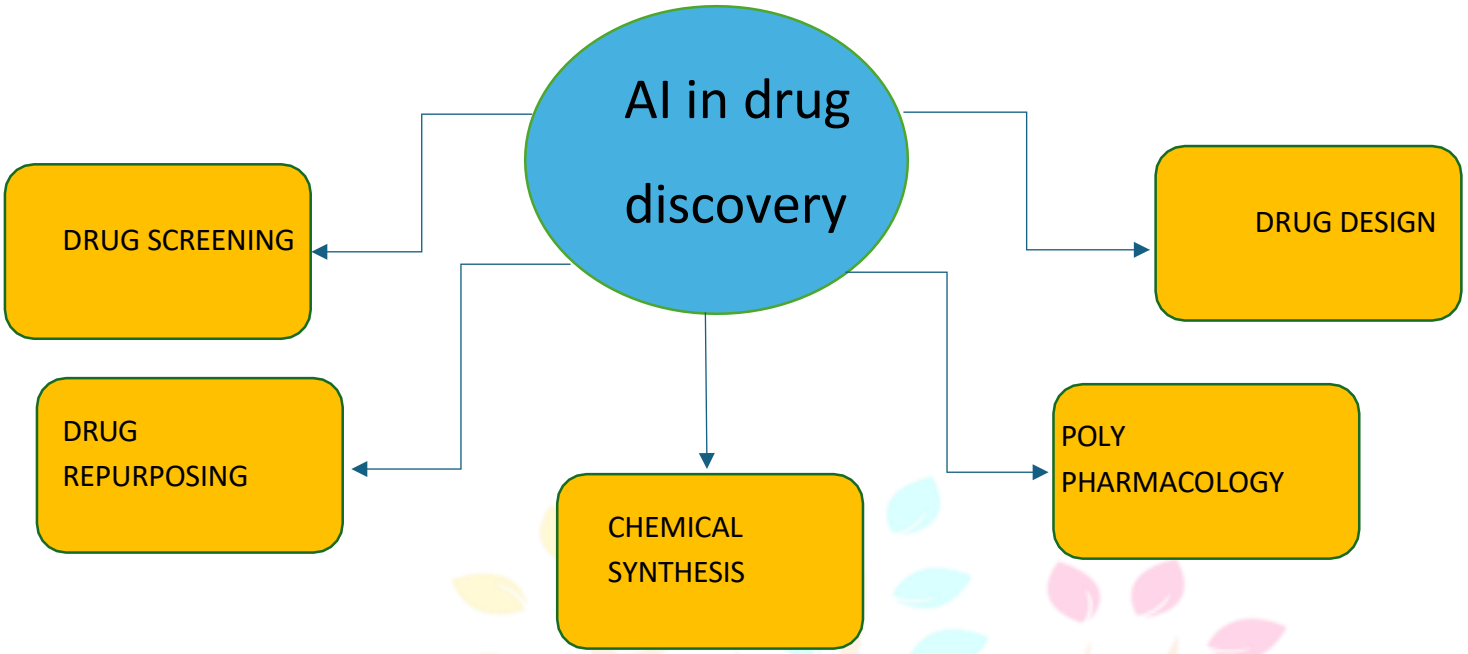


Artificial intelligence (AI) :-

This motivates the uses of AI because It can operate large volumes of data with enhanced automation.AI is a transformation technology-based system involving various advances tools and networks that can imitate humans intelligence. At the same time, it does not replace human presence completely.

The application of AI in drug discover: AI can be used effectively in different parts of drug discovery, including drug design, chemical synthesis, drug screening, poly pharmacology, and drug repurposing. In pharma field, where funding is challenging, return on investment may be insufficient and there

is high need. Computational approaches can provide a lower cost approach for refined the scope of compounds to be tested invitro and in- vivo.



AI based disease identification-

AI is very potential in identification of many infectious disease. AI analyze large amount of data from various sources like: Electronic Health Record, news reports, as well as social media, it quickly detects infectious disease and provides early warning system. AI also predicts the spread of various diseases by determining their population and tracks the movement of individuals. Due to this capacity, AI can significantly improve our ability to identify and response to infectious disease.

In previous years, AI has shown remarkable progress in diagnosis of disease, revolutionizing the way healthcare is delivered.Drug Development

Drug development is a transforming process to identify a new drug and bringing a new pharmaceutical drug from discovery to the market. It includes enhance the process of testing, improving, pre-clinical research on micro-organisms and animals and approving of new drug

. In this process needed to make sure the safe, effective and good quality of drug for receiver.

Key points of Drug Development:-

AI used in Drug Development:

AI has advanced a lot in pharmaceutical research in a new era of drug development and transforming medicine discovery, testing and patient delivery.

Drug development is elaborate and time-consuming process that relies on the experience of drug developers and many trial-and-error experimentation.AI driven the drug development has already meaningful enhancement in both the efficiency and effectiveness of this process. AI technology can identify biomarkers associated with drug response or disease progression, further improving targeted therapies with high efficacy and less adverse effects.

AI-driven drug development can transform the pharmaceutical industries by optimizing preclinical research, clinical trial design and personalized treatment. Researchers profit from AI immediate the discovery, development and delivery of innovative therapies that unmet clinical needs and improve patient outcomes.

Key application of AI in Drug Development:

1- Target identification and validation
2- De Novo Drug Design/Molecule Generation
3- Virtual Screening
4- Predicting Pharmacokinetic and toxicity
5- Drug Repurposing
6- Optimizing Clinical trial
7- Translation Medicine

Real world examples of AI in drug development

1- Nabla Bio – Takeda collaboration

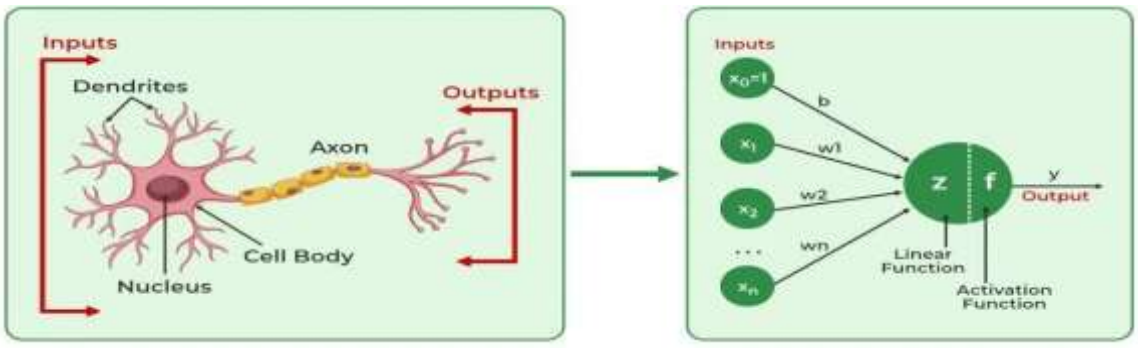
Partnership AI application- JAM is a generative AI model that can design novel proteins (e.g. Antibodies) de novo. Takeda will use this across **- Nabla** bio has expanded its collaboration with Takeda to use its AI platform (**called JAM -Joint atomic model**) for designing protein-based therapeutics, including antibodies.
multiple early stage programs, including challenging targets and multi- specific therapeutics .

2- Isomorphic labs/Alphabet (DeepMind)

Funding and growth :- Isomorphic Labs(An Alphabet/ DeepMind spin- off**) raised $600 million in 2025 to scale its AI- driven drug discovery business.**
The company plans to have **its first AI- designed drug enter humans trials by end of 2025,according to its leadership.**
Significance:- AI not just as a discovery tool, but as a **core engine driving real, human- tested drug candidates.**

AI Networks and tools:

Ai including different methods domains, like reasoning, knowledge representation, solution search and machine learning (ML) . ML uses methodology that can recognise patterns within a set of data that has been these are further classified. A subdivision the ML is Deep Learning(DL), which is engages artificial neural networks(ANNs). ANNs is a series of
algorithms that are recognize underlying relationships in a set of data through a process that mimics the way the human brain operates.
ANNs compose a set of nodes, all receiving a different input, In the end, transforming them to output. Different types of ANNs networks including, Multilayer perceptron (MLP)
networks, recurrent neural networks (RNNs) and convolutional neural networks (CNNs),which are utilize any of supervised training procedure.Fig: Biological Neuron to Artificial Neuron.



The structure of a Biological Neuron: A biological neuron is the basic functional unit of the nervous system. A biological neuron receives, process, and transmit information through electrical (impulses) and chemical signals (neurotransmitters).

- Its input signals from other neurons through, dendrites are receiving signals. Likewise, a perceptron receives its data from other perceptron through input neurons that take numbers.
- In a biological neuron, the output signal is carried away by the axon. Likewise, the axon in a perceptron is the output value which be the input for the next perceptron. Biological neuron is a real messenger in the brain. The function is same (receive – process- output), but mechanism is different (chemical signals vs mathematical operations).

How it work-
Signals received → processed → action potential→ neurotransmitter release→ next neuron activated.

The structure of a perceptron (ANNs): It is a mathematical function used in machine learning. ANNs designed to mimic the function of biological neuron.
In some contexts, the bias, b is denoted by w0. The input, x0 always takes the value 1. So, b1= b.

A perceptron takes the input, x1, x2, …, xn, multiplies them by weights, w1,w2, ... wn and adds the bias term, b, then computes the linear function, z on which an activation function, f is the applied to get the output, y.

Formula:
y= f (w1x1+w2x2+…+)
How it works:
Input weights → added → passed through activation function → output generated.

Artificial neurons vs Biological neurons:

Aspect	Biological neurons	Artificial neurons
Structure	**Dendrites:** Receive signals from other neurons.	**Input node:** Receive data and pass it on to the next layer.
	Cell Body (soma): Processes the signals.	**Hidden layer Nodes:** Process and transform the data.
	Axon: Transmits processed signals to other neurons .	**Output Nodes:** Produce the final result after processing.
Connections	**Synapses**: Links between neurons that transmit signals.	**Weights:** connections between neurons that control the influence of one neuron on another.
	Synaptic Plasticity: Changes in synaptic strength based on activity over time	**Backpropagation:** adjust weights based on errors in predictions to improve future performance.
Activation	**Activation:** Neurons fire when signals are strong enough to reach a threshold.	**Activation function:** Maps input to output, deciding if the neuron should fire based on the processed data.

AI software and used in drug discovery and development

Here's a detailed list of top AI software and platform used in drug discovery and development.

1) Benevolent AI- It uses large biomedical datasets and machine learning to discover new drug targets and repurpose existing drug for different disease, including neurological disorders and COVID-19.

2) DeepMind's AlphaFold-It revolutionized the understanding of protein structure by accurately predicting their 3D shapes. This advancement helps researchers identify potential drug targets with high precision.

3) Insilico Medicine- Insilico medicine, has developed the *apharma.AI* platform that integrates multiple tools such as *panda0mics* for target discovery and *chemistry42* for generating new molecular structure, making it a complete AI-driven drug development ecosystem.

4) Atomwise- It employs its deep learning system called *Atom net* for structure-based drug design, predicting how small molecules will bind to specific protein targets, which vital for identifying promising drug candidate

5) Deep Mirror- Deep Mirror is another AI-driven platform focused on augmented hit-to- lead (H2L) optimization; it helps medicinal chemists improve molecular properties like potency and safety by suggesting optimal chemist modification**.**

6) Ex Scientia-It takes automation even further by designing molecules using AI and bringing AI-generate drug candidate into clinical, trials, showcasing how machine learning can shorten the entire drug discovery process**.**

7) Recursion pharmaceuticals- Combine AI with high – throughout cellular imaging to uncover new uses for existing drugs and explore novel biological pathway.

8) Bio Xcel Therapeutics- It applies its *EvolverAI* platform for drug repurposing and clinical trial optimization helping accelerate the transition from discovery to patient treatment.

9) NVIDIA'S Bionemo and Clara discovery – Its frameworks use generative AI and GPU–powered stimulation to design new molecule and model protein –ligand interaction with remarkable speed and accuracy.

10) Cyclica- It now part of recursion, specializes, in predicting how a single drug might interact with multiple protein targets using its matchmaker platform, aiding in the understanding of drug side effects and polypharmacology.

11) Valence labs and Genesis Therapeutics-It employ graph neural networks to predict important molecular properties, including absorption, distribution, metabolism, excretion and toxicity, which are crucial for evaluating drug safety and effectiveness.

Together, these AI systems are reshaping the pharmaceutical industry by making drug discovery faster, cheaper and more precise.

Challenges and Ethical Considerations:

DATA QUALITY AND PREJUDGMENT IN AI MODELS:

Esurance of the quality and reliability of the data which is obtained by AI models is crucial for accurate prediction and decision making. Incompleteness in data can lead wrong result. AI can inhibit the incompleteness in present training data, which leads wrong prediction or decision. Development of technique for identification and reduce biases in AI models, and ensuring representative training data sets, are important for ethical application in drug discovery.

INTRUPTIBILITY AND TANCEARENCY:

Various AI models, mostly deep learning models, are considered as "black boxes" because their internal working is uninterrupted by humans. This lack of transparency leads concern about how decision is made and compromise trust on AI models. There is a growing need of understandable AI models, where the reasons behind predictions can be understood by people in regulatory authorities. To maintain ethical standards in drug discovery, establishment of mechanism to ensure responsibility for AI based decision, also include transparency and validation of training models is important.

REGULATORY AND ETHICAL IMPLICATIONS:

Application of AI in drug discovery must follow regulatory requirement by agencies, like the Food and Drug Administration and European Medicines Agency. Ensured compliance with regulation designed for traditional drug development processes present challenges due to unique nature of AI technologies. To demonstrate the efficacy and safety of AI generated drug candidates is necessary of regulatory approval. Robust validation and procedure testing is essential to reduce the risk in patients. AI applications, protects patient privacy and secure sensitive data relates to healthcare.

These challenges and ethical consideration are crucial in the responsible and ethical use of AI in drug discovery and development. Collaborative efforts with researchers, regulatory authorities and ethicist in essential to produce guideline that promote ethical uses of AI while maximizing its potential benefits in healthcare.

Ethical legal and regulatory compliances:

Artificial intelligence is at the centre of attention according to its potential benefits in drug discovery such as: reduce cost, decrease timelines and risk alleviation. AI systems can influence critical prediction drug target interaction, toxicity prediction, clinical trials designs, identification, optimisation and pharmacokinetics.

Regulatory platforms align with strict regulatory standard to ensure data integrity, patient safety, customer satisfaction and ethical compliances to fully utilise AI for influence drug efficacy, toxicity and safety. Regulatory bodies like: FDA (Food Drug Administration), EMA (European Medicine Agency) are founded multiple frameworks addressing strict information management criteria.

These are many frameworks includes:

- **21CFR Part11:** Emphasis on the reliability and integrity of electronic records.
- **FAIR Principles**: Findable, Accessible, interoperable and reusable.
- **ALCOA and ALCOA+:** Data management must comply with Good Manufacturing Practices (GMP), Attributable, Legible, Contemporaneous, original and accurate.
- **The Annex11(EU EMA):** Emphasis on software and platform validation, audit trails, and electronic signature.
- **API (Application Programming Interface) :** These are computerized platforms must maintain secure data exchange, traceability, documentation and version control.

The OQ (operational qualification): Operational qualification address the importance of durability, reproducibility of computer platform.

FDA Guidelines for AI in drug discovery and drug development:

FDA approach to AI in drug discovery and drug development focused on ensuring model credibility and trustworthiness through a risk- based, seven- step, framework, Transparency for reliable AI models supporting safety/effect, risk assessment, develop a credibility plan, execute the plan, documentation result and deviation, and ensuring the model's adequacy for its context of use (COU).

Key stages and FDA guidance:

1- Discovery and Development:

In this process, The researchers discover new drugs and identifying a compound for development , these are

including:

- Many testes of Molecular compounds finds to provides beneficial effect against any of a large number of disease.
- The best Administration to give the drug like By mouth or injection.
- How it affects different groups of people (such as by gender, race, Body temperature, weight etc).

2- Preclinical Trails:

The two types of preclinical research are including:

In-vivo: FDA required the researchers to use good laboratory practices(GLP).

In- Vitro: It helps to determine a drug safe, effective and worth testing, in animals or humans.

AI in Toxicity prediction:

FDA requires that:

In- silico toxicity models must be supported with in-vitro and in-vivo confirmation.

AI – generated data must be GLP compliant:

All AI – driven toxicity or PK/PD simulations must including:

Good Laboratory practices (GLP) standards.

ICH M3 (R2): Non clinical studies.

3- Clinical Trials:

FDA Requirements:

- AI used for patient selection must be bias tested.
- AI used in dosing decision must be validated in controlled studies.
- AI based monitoring must ensure data integrity and privacy.

Use of AI in clinical trial design:

ICH E9 (R1): Estimation and statistical analysis. Clinical Trials (Phases 1,2,3):

Phase 1: In this phase, Small group , Focused on safety, dosing .

Phase 2: Larger group, check effectiveness, monitor adverse reactions.

Phase 3: Large scale, focused on confirm effectiveness, monitor adverse reaction.

4- New Drug Application (NDA) and Food Drug Administration(FDA) Review and approval:

NDA: The goal of NDA are request FDA approval to market the drug.

After that all preclinical and clinical data ,manufacturing processes, monitor adverse reactions.

FDA: The process of FDA Review and approval , FDA team receives document to check safety, effectiveness, risk/ benefits, and manufacturing quality. And then complete Response letter or Approval letter.

5- Post Market (Phase -4): The goal of post market, ongoing monitoring of safety and effectiveness after approval.

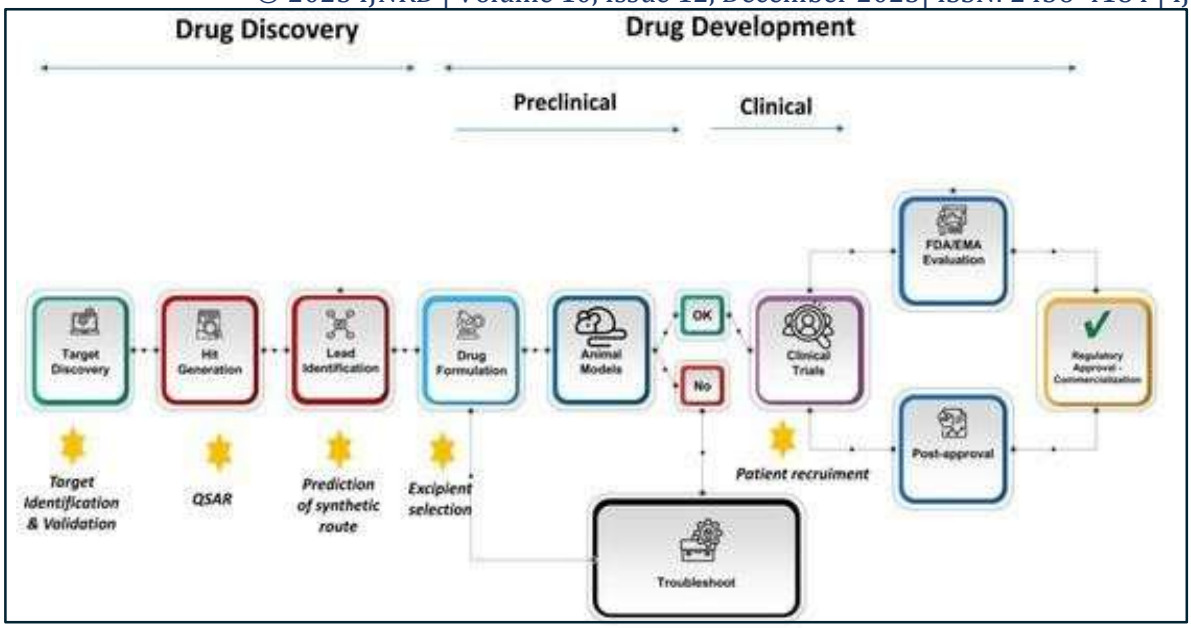


Fig : FDA approval for AI in Drug Discovery and Drug Development

Future Directions and innovations:

Advancements in AI technologies:

Deep learning is the advanced machine learning which could be applied in drug discovery. It is neural network that can extract information form public databases and create scientific conclusion. Deep learning can reduce the costs of clinical trials by predicting their outcomes before the trial starts. Another promising application of AI in drug discovery is drug repurposing. Developing new application for already existing drug reduce their time and cost of development. Some other new trend in the field of drug discovery and development is, application of AI in nanotechnology, mostly as nanocarriers. AI is potential in smart drug release system which deliver the medicine where needed.

Potential impact on drug development:

AI technology can speed up the drug discovery and development process and reduce cost. The resources not dedicated to drug discovery could be inverted into searching of drug for different disease. This could have large impact on public health.

FUTURE OF AI IN DRUG DISCOVERY:

The pharmaceutical industry is increasingly accepted the significant financial burden and potential difficulties associated with traditional Virtual Screening (VS) method. This shifting in approaches is denoted by the remarkable growth of AI market, which reach from $200 million in 2015 to $700 million in 2018. Projection indicates a further rise to $5 billion by 2024; AI is potential in reshaping the pharmaceutical and medical sector. This predicts 40% growth from 2017 to 2024 highlights the profound impact of AI on these domains.

CONSIDERATION FOR SMALL AND LARGE PHARMACEUTICAL COMPANIES:

Customization of AI tools:

Some small pharmaceutical companies may have benefit from customizable AI tools; they are adapted to their specific research needs. The process of customization allows them to focus on there targeted area of drug delivery where most values are provided by AI.

In other hand large companies may have the resource to develop complex AI platforms that can be customise for various stages of drug discovery and development, from target identification to clinical trials.

Resource allocation and return on investment:

The small pharmaceutical companies must carefully allot limited resource before the invest in AI technologies. Company needs to assess the potential return on investment in AI tools and prioritize project. In large pharmaceutical companies, as they have greater financial resource and they can allot significant budget to AI technologies. However they also face pressure to determine appreciable return on investment and ensure that AI investments align with strategic business objectives.

Global Collaborations and data sharing:

The small pharmaceutical companies may have lack of access to large dataset which is necessary to train AI models. To provide access to datasets company should collaborate with academic institutions, research organisations, and some time large companies also, which facilitate more effective AI applications. On other side, large companies often have expensive datasets, but they also it is beneficial to collaborate with external partners. Engaging with global collaboration and data shearing allows them to access more resources, which validate AI models across divers population and accelerate the process of drug discovery.

Both small and large pharmaceutical companies can use AI in drug discovery and development, but some considerations like, customisation of AI tools, resource allocation and global collaboration may differ based on their size, resource and some organisation capability.

Limitations of AI in drug discovery and development:

1) Data related limitation:

a) Poor data quality: AI depends heavily on high-quality datasets, and less depend on biological and chemical datasets.

As data are collected from different laboratories in drug discovery, so they may vary in processing and instrumentation, which leading to batch effect, that compromise reliability of AI prediction.

b) Insufficient data availability: Access to exclusive data remains one of the biggest barriers. As pharmaceutical companies keeps their high-value datasets private due to competitive and financial reasons.

c) Data partiality: Datasets which are used for training may not show the full multiplicity of chemical and biological space. Data partiality can leads the datasets unpredictable, such as overestimating the efficacy of certain compound.

2) Biological complexity and scientific limitation:

a) Incomplete biological understanding: AI applications can only detect pattern in the data that are given but our understanding of biological system is still incomplete. Biological networks involves:

- Nonlinear interaction
- Feedback loops
- Dynamic response to environmental variables

b) Poor translation from in silico to in vivo : Even when AI successfully predict interaction in silico (computer simulation), these result often fail to translate to: In vitro cell system
Animal model Human clinical trials

This translational gap is due to the complexity of living organism, where factors like metabolism, immune, response and genetic variation play critical role that AI cannot fully model.

3) Model related limitations:

a) Overfitting and poor generalization: Many AI models perform unusually well on training data but fail on unseen datasets. This overfitting occurs especially when:

- Datasets are very small
- Chemical structure in the training sets is very similar

- Models are very complicated relative to available data

In drug discovery, this means that predicted hits many look promising in silico but fail in practical testing.

b) Black Box Nature of AI model: Deep learning models often produce prediction without clear explanation. In a field where scientist must justify decision about molecule selection, safety, toxicity and efficacy, this lack of interpretable become a major limitation. Regulatory agencies like the FDA require transparent reasoning for decision making which may current AI tools cannot provide.

c) Limited coverage of chemical space: The chemical universe contains an estimated 10^{60} posible molecule- for beyond what any AI model can explore and train. AI typically works within limited chemical libraries, reducing its ability to discover truly novel molecular structure.

4) Practical limitation in drug discovery pipeline:

a) Need of experimental validation: AI generated projections must still undergo expensive laboratory testing AI cannot replace-

✓ Chemical synthesis
✓ Biological assay
✓ Animal studies
✓ Toxicity screening
✓ Pharmacokinetic testing

This means AI speedup early discovery but does not eliminate the time consuming and expensive experimental workflow.

b) Integration challenges: Drug discovery involves multi-disciplinary term- Chemist, biologist, data scientist, clinicians. Integration AI output into traditional process flow can be difficult due to-

✓ Uniformed data format
✓ Lack of standardization interfaces
✓ Resistance or scientist unfamiliar with AI tools.

c) Slow absorption in regulatory framework: Regulatory bodies need scientific evidence, and AI generated predictions are often contemplated supplementary.
lack of clear guidelines for AI based drugs design slows absorption.

5) Limitations in key drug design tasks:

a) In accurate ADMET prediction: ADMET properties (absorption, distribution, metabolism, excretion, toxicity) are among the most challenging aspect if drug design.
Even advanced AI systems struggle with-

✓ Forecast metabolic pathway
✓ Identifying long term toxicity
✓ Modelling interaction with complex biological barriers

These failures can cause late-stage drug attrition, costing companies millions.

b) Challenges in protein structure and dynamics: Tools like AlphaFold predict protein structure but not-

✓ Protein movement over time
✓ Conformational challenges
✓ Ligand induces structural shift
✓ Interaction in physiological conditions

Drug binding frequency depends on these dynamic processes limiting the utility of AI based structural

predictions.

6) Economic, ethical and social limitations:

a) High computational and financial cost: Training large AI models require-

- ✓ Specialized hardware (GPUs, TPUs)
- ✓ High energy consumption
- ✓ Expensive software and licensing

This makes advanced AI unreachable to smaller research groups.

b) Ethical and security concern: AI can potentially be used to design harmful biological agent or toxic compounds.
This dual use risk demands careful regulation and oversight.

7) Clinical trial and real world limitation:

a) Difficulty modelling human volatility: AI struggle to account for-

- ✓ Genetic diversity
- ✓ Age related difference
- ✓ Comorbidities
- ✓ Environmental factor such as lifestyle or diet.

b) Limited predictive power for clinical outcome: AI cannot yet reliably predict-

- ✓ Long term side effect
- ✓ Real world drug adherence
- ✓ Response in diverse ethic population
- ✓ Rare adverse drug reaction

So, AI plays only a supportive role in clinical trials design, not a predictable one.

Conclusion:

This review showed that AI can revolutionize drug discovery and drug development very well.
AI prospects in the drug discovery and drug development are promising, achieving its widespread applications and in-depth drug discovery and drug development.
Methods based of AI techniques are being adopted in health care industry. Some AI methods like- Low- cost, Intelligent and flexibility are affecting various areas like- Drug design, Support for clinical decision making, Prevention, Diagnosis etc.
AI can immediate target the identification, optimize lead compound and also predict the toxicity and pharmacokinetics of the compound.
By acknowledging the essential challenges, also including insufficient resources and model on large scale, this review demonstrate need of strong validation and ethical consideration in AI derived drug development .
Nevertheless, the future demonstrate requiring need for industry and research community who collaborate to overcome these problems .

The full potential of AI to drive innovation and improve patient outcome in medical research.
AI has transformed early stage drug discovery by speed up task like target identification, virtual screening, and molecular property predication.
How ever it remains limited by-

- ✓ Inadequate data quality
- ✓ Inadequate data availability
- ✓ Biological complexity that model cannot fully compute.
- ✓ Bad generalization and lack of interpredictability.

✓ Regulatory and ethical and economical barriers.
✓ An irreplaceable need for experimental validation.

Eventually, AI cannot replace the drug discovery pipeline; it can only enhance human expertise.

The future of drug discovery will depend on integrating AI with strong scientific understanding, high quality data and strict experimental validation.

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