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ROLE OF AI IN DRUG DISCOVERY – A REVIEW

P Sowmya , Miss. B. Swapna , Mr. M Gurava Reddy, Dr.K.Venugopal
Department of Pharmaceutical Chemistry, Krishna Teja Pharmacy College, Chadalawada Nagar, Renigunta Road, Tirupati -517506

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Abstract:
Recently artificial intelligence has been to be applied more widely in many facets of society, with the pharmaceutical sector leading the way in regard. The effective usage of artificial intelligence (AI) in multiple areas of pharmaceutical industries, drug research and development, medication, repurposing enhancing pharmaceutical production effectively. Consequently, the human workload is reduced and goals are met quickly. The drug discovery is essential to treat new viruses or disease by medications or by developing new drug related to disease. Artificial intelligence aids in drug discovery under COVID-19 in emergency situation. The COVID- 19 pandemic necessitated rapid therapeutic development (BioNTech, Moderna, SARS-CoV-2). Thus reducing the time and cost association with trial- and- error synthesis. Artificial intelligence significantly advances our ability to design and develop safer and more potent drug marking a transformative shift in the landscape of chemistry and pharmaceutical research. Revolutionary progress is expected when artificial intelligence is incorporated into a contemporary, evidence- based drug discovery platform. The AI-based tools are Deepchem, IBM Watson, Alphafold, Shrouding's Maestro, GANs, ChEMBL and Pubchem, GENTRL, HER, Cortellis. These AI tools are reshaping drug discovery by making processes faster, more cost-effective, and less prone to error.

Keywords: *Artificial intelligence, machine learning, deep learning, drug discovery, drug design, AI-driven, drug repurposing, lead optimization, AI tools.*

Corresponding author:
P Sowmya,
Department of Pharmaceutical Chemistry,
Krishna Teja Pharmacy College, Chadalawada Nagar,
Renigunta Road, Tirupati -517506

QR code

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INTRODUCTION:

The integration of artificial intelligence (AI) in drug discovery processes has ushered in a new era of innovation [1]. Artificial intelligence (AI) has the potential to transform the drug discovery process by increasing efficiency, accuracy and speed. The effective use of AI depends on the availability of high-quality data [2]. The AI is having a profound impact on drug discovery. AI is being applied at several phases of the drug discovery process. The utilization of artificial intelligence (AI) is used to new innovation. Critical component of drug discovery including as drug design, Chemistry synthesis, drug repurposing and drug screening are being streamlined and innovatively approached through the use AI technology in drug discovery [3]. A fresh period of innovation has been brought about by the combination of artificial intelligence (AI) with the creation of innovative medications, which has profoundly changed many aspects of drug distribution and discovery. Over the last few decades, pharmaceutical firms have used a variety of AI-related approaches, including as machine learning, deep learning, and other sophisticated computational methods. This has led to previously unheard-of possibilities for the advancement of the medication delivery and discovery processes, which in turn has improved patient outcomes and optimized treatment plans. we define several terms related to drug discovery primary those related to small molecules design and screening it should be noted that AI-powered medication repositioning is excluded. The method repurposes current medications or prescription combination for novel indications. Additionally, target identification that is using omics data to determine if a target can be treated-is outside the purview and is not included. Instead, we direct the readers to earlier works on medication reposition and omics data for target determination [4].

Drug discovery in the AI era:

The application of AI in drug discovery is widespread. Machine learning methods, such random forest (RF), have been used for VS and QSAR since the early 2000s [5]. Soon later, deep neural networks (DNNs) beat the conventional RF model in the 2012 Merck Kaggle competition when it came to predicting chemical activity [6].

This survey focuses on lead identification, which entails two core tasks: molecule creation and chemical property prediction. Predicting a molecule's property value based on its structure or learned representation is the fundamental function of virtual screening (VS) and can be applied to a number of scenarios, including Drug-induced liver damage (DILI), toxicity, and drug-target interaction (DTI) predictions [7]. Creating molecules within the limitations set by chemical principles is known as realistic molecule generation, and creating chemically valid molecules with desired qualities is known as goal-directed molecule generation. These tasks are the foundation of drug design.

AI in Drug Repurposing:

Drug repurposing, often known as drug repositioning or re-tasking, is the process of finding new therapeutic uses for medications that were once created to treat different medical ailments. Compared to conventional drug discovery pipelines, this strategy has attracted a lot of interest since it offers the potential to expedite the process of developing drugs, save costs, and deliver pharmaceuticals to patients more quickly [8]. AI facilitates the repurposing of drugs using a variety of techniques, such as feature-based, network-based, and matrix-based methods. Given the known safety characteristics of these drugs from earlier studies, one major advantage of AI-driven drug repurposing is avoiding early-phase clinical trials and toxicological evaluations. This effectiveness significantly shortens development times and costs by enabling repurposed medications to move straight to Phase II trials for novel indications [9].

AI-Based Tools in Drug Discovery:

The rapid growth of artificial intelligence (AI) technology has the potential to revolutionize drug discovery by facilitating researchers' ability to effectively explore extensive databases, devise novel chemical structures, and forecast the effectiveness of prospective therapeutic candidates**.** The tools are Pubchem, AlphaFold, IBM Watson, DeepChem, DeepTox, drug bank, Organic, Hit Dexte [10].

AlphaFold:

It is extremely difficult and complex to predict the three-dimensional structures of proteins based on their amino acid sequence. AlphaFold, created by DeepMind, is publicly accessible through Google Colab and has attained a record-breaking degree of accuracy [11].

DeepChem:

Tensorflow wrappers that comprehend and simplify the processing of chemical datasets include the DeepChem library. For drug discovery and application tasks such modeling BACE-1 inhibitors, it has been utilized for algorithmic research into one-shot deep-learning algorithms. DeepChem may be used to count the number of cells in a microscopic picture, estimate

the solubility of small molecule medications and their binding affinity to targets, and study protein structures. The DeepChem package now includes MoleculeNet , which has the characteristics of 700,000 chemicals[12].

DeeperBind:
Modeling the interaction between transcription factors (TF) and their corresponding (DNA/RNA) binding sites, DeeperBind is a long short-term recurrent convolutional network that predicts protein binding specificity in respect to DNA probes. DeeperBind is capable of accurately forecasting probe sequence dynamics [13]. Additionally, datasets with sequences of varying lengths can be used for testing and training.

PubChem:
With over 111 million compounds, 279 million substances, 295 million bio-activities, and 34 million articles arranged into three interconnected online data pages substance, compound, and bio-assay PubChem is the biggest free collection of chemical knowledge. The bio-assay database contains the test results and descriptions of bio-assays. To find chemicals for a certain target or protein, data mining techniques might be applied [14].

ChEMBL:
The European Molecular Biology Laboratory (EMBL) created the open-access drug discovery database ChEMBL. Data on tiny compounds and their biological activity are merged with information on approved and potential drugs, including their mechanism of action and therapeutic indications, which are collected from full-text articles in high-impact journals. The bioactivity data is shared with other databases, including PubChem Bioassay and BindingDB. To find chemical tools for a target of interest, forecast drug-target interactions, repurpose a drug, assess target tractability, and integrate with current drug discovery tools, the ChEMBL database has been utilized [15].

DrugBank:
DrugBank offers clinical information, side effects, medication interactions, repurposing, and molecular-level data. It is extensively utilized for machine learning-based drug discovery, repurposing, and *in silico* drug design [16].

Automation in Chemical Synthesis (AI):
Chemical synthesis, optimization, and discovery automation methodologies have often been developed with an emphasis on engineering solutions to real-world issues rather than taking into account the constraints of laboratory-based research [17]. This is due to the fact that while organizing a synthetic process, organic chemists frequently think both ahead and backward. The creation of a universal chemical method utilizing a programming language with automation in conjunction with machine learning and artificial intelligence (AI) is the answer to this issue, as demonstrated in this opinion piece [18].

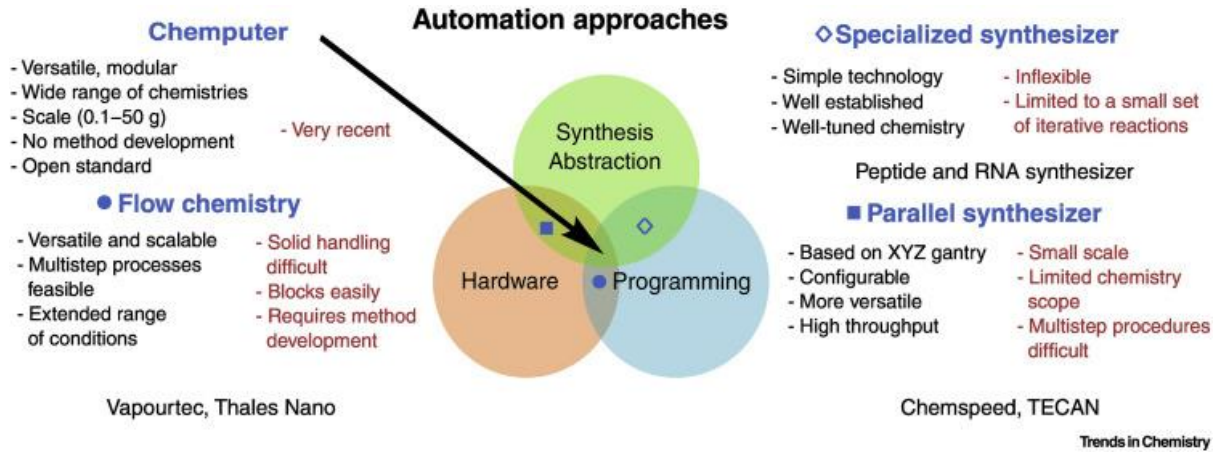
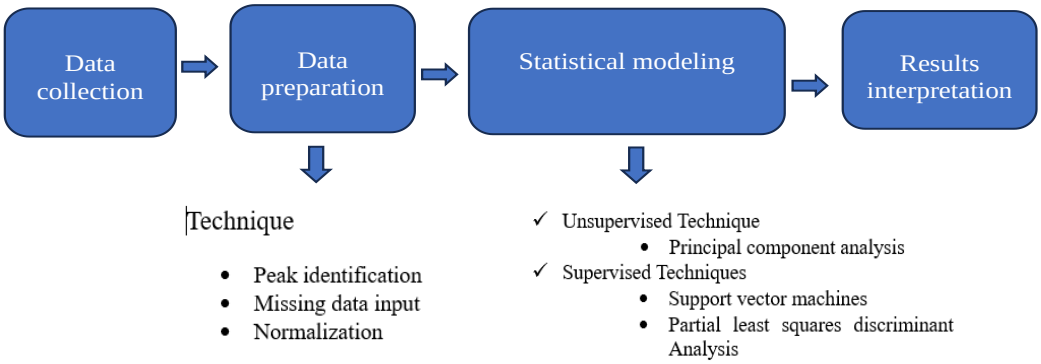


Fig.1: Automation approaches in chemical synthesis

PROCEDURE FOR AUTOMATION APPROACHES



Applications in drug discovery:

- Prediction of Molecular Properties: AI models forecast crucial molecular characteristics that are essential to medication effectiveness, such as permeability, stability, and solubility [19].
- Relationship between Structure and Activity (SAR) Modeling: By identifying correlations between chemical structures and biological activity, machine learning approaches aid in the development of more effective medication candidates [20].
- De Novo Drug Design: By recommending new synthesis options, AI algorithms optimize drug development by creating unique chemical structures with desirable biological features [21].
- Reaction Prediction: AI assists synthetic chemists in devising effective pathways for the synthesis of medicinal molecules by forecasting the results of chemical reactions, including retrosynthesis [22].
- The relationship between quantitative structure and activity, or QSAR Modeling: Chemical structure and biological activity are correlated using AI-based QSAR models, which shed light on the safety and efficacy of medications [23].
- Drug-Like Property Optimization: AI aids in the refinement of compounds to guarantee that they possess drug-like characteristics, including the right molecular weight, lipophilicity, and bioavailability [24].

CONCLUSION:

By lowering development costs, increasing prediction accuracy throughout the process, and speeding up the identification and optimization of new drug candidates, artificial intelligence (AI) holds the potential to completely transform drug discovery. AI-driven solutions optimize processes from target discovery to clinical trials, allowing for quicker, more informed decision-making. Drug development is becoming a more productive and efficient process thanks to the increasing synergy between AI and human skills, despite obstacles including data quality, ethical issues, and model interpretability. As AI technology develops, it has the potential to open up novel treatments, giving hope for more rapid, cost-effective, and individualized care that will eventually improve healthcare worldwide. There is also discussion on the future of artificial intelligence in the pharmaceutical sector, current obstacles, solutions and the methods and instruments used to enforce artificial intelligence (AI). AI can speed up target identification, enhance lead optimization, forecast drug interactions, and eventually bring successful medications to market more quickly by utilizing enormous volumes of biological and chemical data.

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