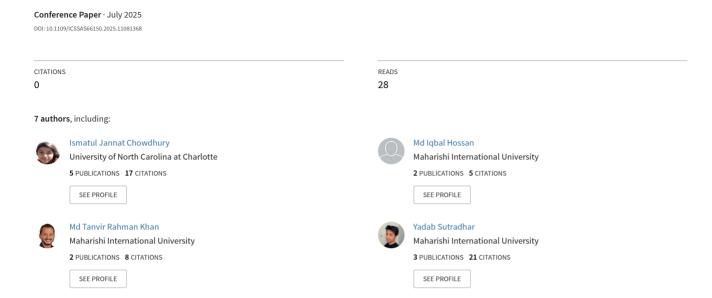
Revolutionizing Drug Discovery: A Systematic Review of AI and Machine Learning Application



Revolutionizing Drug Discovery: A Systematic Review of AI and Machine Learning Application

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Abstract—Artificial intelligence (AI) and machine learning (ML) have transformed drug development, tackling issues like poor clinical trial success rates, high prices, and extended timescales. Target discovery, lead optimisation, drug repurposing, and toxicity prediction—among other aspects—of artificial intelligence and machine learning's influence across drug Examining more than 15 current development phases. investigations, the review emphasises new methods and constraints. Deep learning (DL) and reinforcement learning (RL) have raised target identification and virtual screening effectiveness, thus improving drug discovery Companies like Sumitomo Dainippon Pharma and Insilico Medicine have shown how artificial intelligence can anticipate medicinal properties, speed lead drug discovery, and reuse already-existing medications. Platforms powered by artificial intelligence like Centaur Chemist and Atomwise have accelerated the search for treatments for illnesses like Ebola and schizophrenia. Still, artificial intelligence implementation must contend with issues like "black-box" constraints, model interpretability, and data quality. Furthermore covered in the research is how Explainable AI (XAI) could increase openness and confidence in AI-driven drug discovery methods.

Keywords—artificial Intelligence(ai), machine learning(ml), drug discovery, target identification, drug repurposing, lead optimization, toxicity prediction.

I. INTRODUCTION

Comprising 10-15 years and costing around \$2.6 billion, the drug development process has a low success rate. Less than 10% of drug ideas survive Phase I clinical trials, which emphasises inefficiency even with significant expenditures [1][2]. Promising better efficiency, lower costs, and higher success rates, this has spurred the acceptance of Artificial Intelligence (AI) and Machine Learning (ML) to simplify and optimise many phases of drug development. A subset of artificial intelligence, ML lets computers learn from massive data sets without explicit programming, transforming several spheres of drug research. Target identification—the vital initial stage in drug development—is especially being changed by artificial intelligence. Analysing biological data including gene expression and protein-protein interactions helps uncover novel druggable targets by use of machine learning techniques, particularly deep learning (DL). Deep learning algorithms have also been used to forecast binding affinity, hence enhancing the hit-to---le phase [7]. AI is improving virtual screening (VS), which from large chemical databases finds interesting drug-like molecules. Although conventional VS techniques are efficient, they suffer with accuracy and efficiency. More robust and accurate AI-driven VR employing Random Forest (RF) and Support Vector Machines (SVMs) lowers false positives [8][9], hence allowing quicker compound prioritising. AI is increasing the potency, selectivity, and bioavailability of drug candidates in

lead optimisation. Generative models, including Variational Autoencoders (VAE) and Generative Adversarial Networks (GANs), develop novel compounds that satisfy certain requirements, therefore quickening the optimisation process and lowering costs [10][11]. AI is also transforming drug repurposing—that is, discovering new applications for already-used drugs. During the COVID-19 epidemic, this was extremely helpful as artificial intelligence rapidly found possible remedies by examining pharmacological databases and scientific literature [12]. Personalised medicine is another area where artificial intelligence has promise as it may suggest treatment regimens depending on medical history and genetic profiles. AI models examine medical imaging in cancer therapy to forecast the best course of action for particular patients [13][14]. AI has difficulties even with great potential. Since artificial intelligence algorithms depend on big, highquality annotated datasets, data quality and availability remain major obstacles. Data silos, inconsistent formats, and missing datasets still plague the pharmaceutical sector. Furthermore, artificial intelligence models—especially deep learning models—are often seen as "black-box" models, which makes it challenging to grasp and believe their forecasts [15][16]. Explainable artificial intelligence (XAI) is becoming popular in order to handle these issues. XAI increases trust and interpretability by clarifying the AI model decision-making process, hence fostering openness. It also improves the dependability of AI-driven drug development by helping to spot mistakes and prejudices [17][18].

By speeding up procedures, raising success rates, and lowering costs, artificial intelligence and machine learning are ultimately changing drug development. Faster medication development and more tailored therapies are possibilities provided by these technologies. To realise their full potential, however, one must overcome obstacles such data quality, model interpretability, and regulatory clearance. AI will become even more important in determining the direction of healthcare as it develops [19][20]. The present situation of artificial intelligence in drug development is investigated in this review along with successes, difficulties, and future prospects.

II. RELATED WORK

AI and ML in drug discovery are revolutionising the pharmaceutical industry. These technologies aim to overcome drug development issues such high prices, extended development times, and high clinical trial failure rates. Looking at thirty studies holistically reveals varied methods, strategies, and conclusions that show how artificial intelligence and machine learning might change medication development.

A. AI Applications in Drug Discovery

AI applications in drug research include target identification, lead finding, lead optimisation, clinical trials, and drug repurposing. Artificial intelligence can evaluate large datasets to discover drug candidates and predict their biological action, saving time and money [21]. DSP-1181, developed by Sumitomo Dainippon Pharma, was the first AI-identified drug in clinical trials. The AI system Centaur Chemist found a promising schizophrenia treatment using machine learning to predict chemical biological properties [17]. This illustrates how artificial intelligence may find novel compounds that traditional approaches overlook, simplifying lead finding.

B. Drug Repurposing Using AI

AI is also promise for medicine repurposing. Atomwise deep learning has uncovered compounds that fight multiple sclerosis and Ebola. Analysing massive amounts of clinical data enables artificial intelligence systems to repurpose drugs for new applications, speeding up drug development [17]. AI-driven systems like Insilico Medicine's GENTRL develop innovative chemicals that may cure illnesses without effective treatments. [19]. Repurposing existing drugs with AI reduces adverse effects since they have been clinically examined.

C. Optimizing Clinical Trials with AI

Artificial intelligence for clinical trial optimisation is another hot topic. By identifying patient groups most likely to benefit from a medication, machine learning algorithms increase clinical testing efficiency [19], reducing trial requirement. Artificial intelligence may identify cancer patients more likely to react to therapy, improving clinical trial success rates [23]. Watson for Drug Discovery developed pembrolizumab. There is still effort to ensure that AI can be utilised properly across numerous communities and diseases. Artificial intelligence's clinical trial potential depends on answering ethical problems about data privacy and the need for large, high-quality datasets.

D. AI in Target Identification

AI is transforming target identification, a crucial step in drug development. Artificial intelligence algorithms may uncover disease-related biological targets by examining genomes, proteomics, and chemical data. For instance, Chinese pharmaceutical technology company XtalPi uses quantum mechanics and AI to predict drug characteristics and interactions, enhancing drug discovery [17]. Artificial intelligence's capacity to analyse molecular and genetic data helps find new disease-target linkages, leading the creation of more effective and safer drugs. These projections primarily depend on the quality and amount of data used to train AI systems.

E. Limitations and Challenges

Despite its promise, AI in drug discovery faces several challenges. One of the primary limitations is the availability of high-quality, standardized data. AI systems require vast amounts of annotated data to train effectively, but in many cases, data is fragmented, inconsistent, or incomplete. Moreover, issues related to data privacy, particularly in clinical settings, make the integration of AI into drug discovery complex and slow [19]. Another challenge is the "black-box" nature of many AI models, especially deep learning algorithms, which make it difficult to interpret the

decision-making process. This lack of transparency raises concerns about the reliability of AI-driven predictions, particularly in clinical settings where decisions can have life-or-death consequences [17].

F. Novelty and Accuracy of AI Models

AI in drug development has several challenges despite its promise. Data quality and standardisation are major constraints. Despite fragmented, inconsistent, or insufficient data, artificial intelligence systems require enormous amounts of tagged data to learn. Data privacy problems, particularly in clinical settings, complicate drug discovery using AI [19]. The "black-box" nature of many artificial intelligence models, especially deep learning algorithms, makes decision-making difficult to explain. This lack of transparency raises worries about AI-driven projections, especially in hospital settings where choices might be life-or-death [17].

G. Future Directions and Plans

Drug development will increasingly rely on AI and ML. Using Explainable AI (XAI), researchers are improving AI system interpretability and transparency. XAI aspires to make AI systems more visible and enhance trust in AI-driven medicine development by providing clear rationale [19]. Future ideas include merging AI with quantum computing to enhance medicine development estimates. This research is being done by companies like XtalPi and might lead to pharmaceutical design and development advances [17].

III. RESEARCH METHODOLOGY

This systematic literature review searched for the most relevant and recent AI and ML drug discovery investigations. PubMed, IEEE Xplore, Scopus, and Google Scholar were utilised to ensure data completeness. Due to their vast variety of healthcare and computer science articles, these databases are ideal for capturing the intersection of AI and drug development. The search for "Artificial Intelligence in Drug Discovery," "Machine Learning in Pharmaceutical Industry," and "AI in Drug Development" yielded publications on AI and ML in medication development. Boolean operators like "AND" and "OR" narrowed the search results and ensured inclusion of research on "target identification," "lead optimisation," and "drug repurposing." For example, "Machine Learning AND target identification" would focus on studies on how ML is used to find new druggable targets, while "AI AND drug repurposing" would focus on articles on how AI is being used to find new uses for existing drugs. This helped focus the findings on the most relevant field research.

The search was confined to the past 5-10 years to ensure the review included the latest findings in AI-driven drug development. Articles on AI and ML techniques in drug development were filtered to exclude generic or unoriginal findings. Research was assessed for its relevance to target discovery, lead optimisation, medication repurposing, and toxicity prediction. [1] [2]. This extensive search helped us assemble a body of data that ensures the review covers the latest discoveries, concepts, and challenges in drug discovery using artificial intelligence and machine learning. [3] [4]. As machine learning is used to solve drug development and

discovery issues, we wish to extensively examine the latest technology, breakthroughs, and academic papers in this field. As seen in Figure 1.

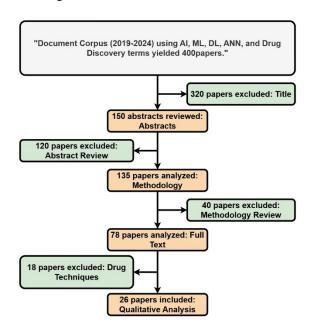


Fig. 1. Criteria of study selection

A. Data Extraction and Synthesis

The data extraction technique for this systematic literature review was to collect and organise key information from the selected studies. Every study's AI and ML techniques, drug development stages, and outcomes were highlighted. Important details included target discovery, virtual screening, lead optimisation, medication repurposing, and toxicity prediction. These steps were selected for AI drug discovery optimisation. For each research, accuracy, AI/ML model success rates, and challenges were recorded. characteristics were crucial to understanding AI-driven model relevance and performance in the pharmaceutical industry [1][[2]. The key data points were sorted into drug development categories such target identification, toxicity prediction, and virtual screening. This categorisation allowed a systematic evaluation of how artificial intelligence and machine learning are used in medication development. For instance, target identification investigations were separated from virtual screening and toxicity prediction research, revealing AI's drug discovery applications [3]. [4]

Data from many studies was compared to identify AI utilisation trends, similarities, and variances. Particularly focusing on how AI may ease drug discovery was This includes examining how AI models are boosting drug development efficiency, cost, and accuracy, especially in virtual screening, where AI can identify potential drug candidates from enormous chemical libraries [5(16.pdf). [6]. Researcher challenges included data quality, model interpretability, and AI integration into pharmaceutical operations [7]. This comprehensive data extraction and synthesis approach provided a holistic view of artificial intelligence in drug discovery, highlighting both its successes and places for improvement. [8] [9].

A. Quality Assurance and Bias Minimization

This systematic literature review prioritised choice and bias reduction throughout data collection and article selection. To verify the authenticity and relevance of the included research, two independent reviewers participated throughout the process. This double-checking ensured the review's integrity and that only studies meeting inclusion criteria were examined. The two reviewers thoroughly investigated and resolved any disagreements by consensus, ensuring consistency and fairness in the final conclusion. [1]. [2]. The research purposely includes publications with different experimental settings and AI methods to prevent selection This strategy used artificial intelligence for target discovery, medicine repurposing, and toxicity prediction throughout drug development. The research covered a wide variety of AI applications by including studies on supervised learning, reinforcement learning, and deep learning models. This spectrum of approaches ensured that the results were not biassed towards any AI method, improving their generalisability and use in the pharmaceutical industry [3]. [4]. Every study's methodological quality was carefully assessed along with its artificial intelligence methods. The evaluation only included scientifically rigorous papers with well-supported results and clear research methods. This process ensured that only scientifically sound and full papers were included in the review. To avoid include irrelevant or methodologically poor publications [5], the research were evaluated based on their relevance to artificial intelligence in drug development. [6]. Through these efforts, the review aimed to reduce selection bias and erroneous findings to ensure that the final synthesis accurately represented artificial intelligence applications in drug development. [7] [8].

B. Data Analysis Techniques

Data analysis was done in this systematic literature review utilising both qualitative and quantitative approaches to offer a complete knowledge of the influence of artificial intelligence approaches on drug discovery. Examining the several artificial intelligence approaches utilised in drug discovery—deep learning (DL), support vector machines (SVM), and reinforcement learning (RL)—was the main emphasis of the qualitative investigation. identification, lead optimisation, virtual screening, and toxicity prediction were among the several phases of the drug development pipeline for which this study sought to evaluate the efficacy and usefulness of each approach. Understanding how various artificial intelligence approaches support these phases helped the review to make judgements regarding which approaches are most successful in improving the drug discovery process and in which particular sectors they are most useful. [1] [2]. Important performance criteria of artificial intelligence-based solutions and conventional drug discovery techniques were assessed and compared using quantitative analysis. Examined to underline the benefits of artificial intelligence integration into the pharmaceutical sector were metrics like accuracy, success rates, computing efficiency, and the lowering of drug discovery times. Studies using artificial intelligence in virtual screening or lead optimisation, for instance, usually found faster, more accurate identification of promising drug candidates than using more traditional techniques. Likewise, the study revealed that AIdriven models drastically cut the time and expenses related to several phases of medication development, including toxicity testing and in silico drug screening. These measurable gains show how well artificial intelligence might maximise the drug

development process. [3] [4]. Combining qualitative and quantitative studies, the study presented a whole picture of how artificial intelligence might affect drug research. While the quantitative study let for objective comparisons of the performance of the several artificial intelligence techniques, the qualitative research revealed insights on their particular applications. This all-encompassing strategy not only emphasises the present capacity of artificial intelligence in drug development but also identifies areas where more research and innovation are required to completely realise its possibilities in the pharmaceutical sector [5] [6].

IV. RESULT ANALYSIS

A. Results

1). Advanced Technologies in Drug Discovery

Modern technologies are being used by the pharmaceutical sector more and more to improve production techniques and medication development. One well-known example is the in silico ADMET (absorption, distribution, metabolism, excretion, and toxicity) system. This platform provides important new perspectives for the creation of drugs since it models pharmacokinetic and physicochemical features. Either direct interactions between chemicals and designated proteins or secondary data can be used to create sophisticated deep learning models assisted by artificial intelligence algorithms. Although the later method involves constant monitoring to guarantee data quality and prevent mistakes [6], it allows for thorough data analysis and can produce quite accurate results even if it is resource-intensive. Blockchain is another really significant technology used in pharmaceutical sector. By building unchangeable records accessible to several stakeholders in the drug discovery and clinical trial procedures, blockchain technology guarantees data integrity and transparency. Tracking drug transactions and clinical studies as well as simplifying the procedure and raising efficiency have found benefit from it. Still, significant implementation and maintenance costs remain a deterrent, so adoption of it is limited mostly to bigger companies [7]. Additionally becoming popular is 3D printing, which provides on-demand manufacturing capacity so less reliance on conventional production techniques is required. Particularly with developments like blue light printing, this technology increases the scalability and precision of drug manufacturing techniques [8].

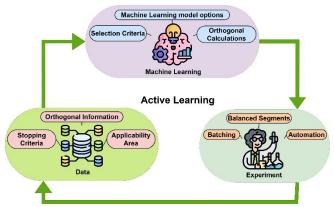


Fig. 2. Machine learning drug discovery [12]

2). Machine Learning in Drug Discovery

Drug discovery is depending more and more on machine learning (ML), which is transforming how pharmaceutical corporations handle R&D. ML has been demonstrated to improve efficiency, lower costs, and expedite the introduction of new medications to market in the context of drug discovery. By simulating and predicting drug interactions, toxicity, and efficacy by means of their integration with high-throughput screening technologies, ML models are especially useful in drug screening, hence lowering the demand for conventional animal testing [10]. Figure 2 shows a simplified cycle of the processes that take place during the use of machine learning in the pharmaceutical industry, especially the manufacturing and development sectors of this indus- try, and also demonstrates how machine learning is generally done [12].

The general acceptance of ML among different pharmaceutical corporations attests to its success and applicability. Drug characteristics including solubility, bioavailability, and toxicity have been predicted, for instance, using ML models. Recursive neural networks and adversarial auto-encoders are among AI-based models used to forecast the solubility of different chemicals, surpassing conventional techniques in accuracy and efficiency [23] [24]. Furthermore, reactions to anticancer drugs have been predicted using ML methods including transfer learning, hence greatly enhancing the predictive accuracy over more traditional models [19]. Crucially important for the drug development process, drugtarget interaction prediction has also benefited much from ML. Simulating biological processes and predicting how new medications will interact with their targets has been done using several ML models, including adversarial networks, multitask learning, and reinforcement learning. Faster and more accurate drug development has resulted from the identification of new drug candidates with greater accuracy and efficacy resulting from this application [25]. Deep learning and multitask learning techniques have been made possible by further developments in ML algorithms to examine large-scale data, enhance drug screening accuracy, and even forecast antibacterial characteristics of various compounds. This combination has produced notable changes in the general dependability of drug discovery techniques and notable decreases in processing times. [26][27]. A compilation of other studies that used machine learning in drug discovery shown in table 1.

TABLE I. A COMPILATION OF OTHER STUDIES THAT USED MACHINE LEARNING IN DRUG DISCOVERY

Study	Techniq	Applicatio	Methods	Accuracy
	ue	n		
Margulis	Machine	Identificati	Machine	80%
et al. [28]	Learning	on of bitter	learning	match with
		molecules	to predict	BATA
		in drugs	bitterness	experimen
				t
Raschka	Machine	GPCR-	Machine	Close to
et al. [29]	Learning	ligand	learning	baseline
		recognition	algorithm	performan
			s for	ce
			ligand	
			discovery	

Pereira et al. [30]	Machine Learning	Drug-target interaction prediction	Machine learning for docking receptor ranking	Higher performan ce than standard ranking
Turki and Taguchi [31]	Reinforc ement Learning	Drug discovery	Reinforc ement learning for drug identifica tion	46 days for discovery
Zhavoro nkov and Mamoshi na [32]	Transfer Learning	Drug response prediction for myeloma patients	Transfer learning to predict responses	Greater predictive accuracy
Provenza no et al. [33]	Deep Learning	Anti- microbial peptide discovery	Deep learning platform for peptide identifica tion	Novel peptide discovery
Yi et al. [34]	Deep Learning	Anti-cancer peptide discovery	LSTM algorithm for anti- cancer peptides	Successful peptide discovery

3). Artificial Intelligence in Drug Discovery

Particularly in the form of machine learning, artificial technologies—especially intelligence are helping tremendously in the drug discovery process. By allowing the prediction of physicochemical features, these technologies help to lower the demand for expensive and time-consuming clinical research. Drug discovery's efficiency and success rates are being much raised by AI-driven methods including polypharmacology and drug repurposing. Mass data handling and machine learning algorithm integration by artificial intelligence have made it feasible to simplify the drug design and drug screening procedures, thereby hastening the path of new pharmaceutical development. [35] [36]. Reducing the dependence on preclinical animal testing, AI-based predictive models are also vital for spotting possible toxicity and pharmacokinetic traits of drug candidates. For example, artificial intelligence models such as eToxPred have shown a high degree of accuracy in predicting the toxicity levels of various compounds, implying that in some cases such AIdriven systems could possibly replace conventional clinical trials [27]. Figure 3 above shows where and how AI can be implemented in drug discovery and development activities and the new uses of AI in the pharmaceutical industry [36].

Another area of continuous research in artificial intelligence applications within the pharmaceutical industry is drug repurposing—where AI systems investigate present drugs and their connections with various diseases, therefore revealing new therapeutic possibilities. Furthermore very promising for treating challenging diseases polypharmacology, in which artificial intelligence forecasts numerous pharmaceutical interactions with a spectrum of targets [37]. of other research that applied artificial intelligence for drug discovery is shown in table 2.

At last, machine learning and artificial intelligence are ready to keep evolving the drug discovery procedure by means of greater dependability, affordability, and efficiency. As technology develops, new ideas will appear and help pharmaceutical companies to manufacture new therapies faster and more precisely, hence increasing their ability Still, the general integration of artificial intelligence and machine learning in the industry depends on overcoming challenges including regulatory frameworks, data standardising, and model openness.

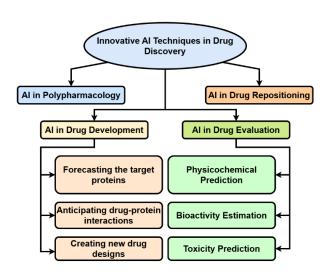


Fig. 3. Application of artificial intelligence in drug discovery[36]

TABLE II. PERFORMANCE METRIC A SUMMARY OF ADDITIONAL INVESTIGATIONS THAT USED AI TO FIND NEW DRUGS

Study	Techniq	Applicati	Methods	Accuracy
,	ue	on		,
Lusci	Recursi	Predictio	Prediction of	More
et al.	ve	n of	solubility of	accurate
[23]	Neural	solubility	chemical/biol	than
	Networ	_	ogical	conventiona
	k		molecules	1 methods
Polyk	Advers	Drug	Prediction of	Very
ovskiy	arial	screenin	activity of	accurate,
et al.	Auto-	g	synthesized	compounds
[7]	Encode		molecules	generated
	r			with novel
				information
Dayna	Artifici	Antimicr	Prediction of	70%
c et al.	al	obial	antimicrobial	accuracy
[38]	Neural	propertie	properties	with low
	Networ	S		error margin
	k			
Pu et	eToxPr	Toxicity	Predicting	72%
al.	ed	predictio	toxicity levels	accuracy,
[39]		n	of compounds	4% error
				rate
Kadur	Advers	Drug	Screening	72 million
a et al.	arial	screenin	anticancer	molecules
[40]	Auto-	g for	molecules	screened
	Encode	anticance		
	rs	r		
		molecule		
		S		
Mara	Various	Predict	Prediction of	71.9%
m and	AI	biologica	drug activity	accuracy,
Hamd	process	1 activity	with cell types	low error
y [41]	es			margin

Zhavo	Transfe	Drug	Predicting	Greater
ronko	r	response	responses to	predictive
v and	Learnin	predictio	drug in	accuracy
Mamo	g	n	multiple	than
shina			myeloma	baseline
[42]				methods
Rasch	Machin	GPCR	Cross-	Performance
ka et	e	ligand	checking	close to
al.	Learnin	recogniti	results from	baseline
[43]	g	on	traditional	
			receptors and	
			machine	
			learning	

V. FUTURE SCOPE

The future of AI and ML in drug discovery is poised for expanded revolution as a consequence of continued growth in computational power, data collection, and algorithm improvement. Amongst these, disassembling the current limitations in data quality, integration, and privacy will be a critical domain of focus, as the latter is continuing to hinder widespread adoption of AI technologies. The emergence of Explainable AI (XAI) will solve the problem of deep learning model opacity, making decisions taken by AI more transparent and interpretable. It will enhance trust levels among stakeholders as well as regulatory approval procedures. Additionally, the integration of AI with newer technologies like quantum computing has immense potential for improving predictive accuracy and computational efficiency, resulting in accelerated drug discovery timelines. Furthermore, expansion of AI within polypharmacology and drug repurposing will unlock new therapeutic applications of existing drugs on the market with faster pathways to clinical trials. Future research would also look to explore generalizability of AI in clinical trials, for instance, personalized medicine, whereby AI models can provide tailored treatment plans based on gene data and other patientspecific features. The collaboration between AI platforms, pharma companies, and regulatory bodies will play a critical role in the smooth integration of AI technologies into drug development. These advancements will eventually result in more effective, targeted treatments, revolutionizing the drug discovery process and improving patient outcomes in the future.

VI. CONCLUSION

This systematic literature review has highlighted the transformative potential of Artificial Intelligence (AI) and Machine Learning (ML) in revolutionizing drug discovery. Despite the traditional drug development process being timeconsuming, resource-intensive, and fraught with challenges, AI and ML offer innovative solutions that significantly enhance efficiency, reduce costs, and improve success rates. Through various applications such as target identification, drug repurposing, lead optimization, and clinical trial optimization, AI-driven models have demonstrated the ability to predict drug efficacy, identify promising candidates, and even reduce the need for traditional animal testing. However, the widespread integration of AI into the pharmaceutical industry faces challenges, primarily concerning data quality, model transparency, and regulatory acceptance. The development of Explainable AI (XAI) has emerged as a critical step toward addressing these concerns, ensuring that AI models are interpretable and trustworthy. Moreover, the combination of AI with emerging technologies like quantum computing holds the potential to further accelerate the drug discovery process. The future of AI in drug discovery is bright, with continuous improvements in computational methods, data availability, and algorithmic advancements. As these technologies evolve and overcome current limitations, AI will play an increasingly central role in the development of more personalized, effective, and efficient therapeutics. The findings of this review underscore the need for further research to unlock the full potential of AI and ML in reshaping the drug discovery landscape

Boosting might still require further tuning for increased processing and performance. On the other hand, Linear Regression, although efficient in computation, presented limitations regarding nonlinear interactions, as it had a rather lower R² score of 0.946. This is in agreement with the work of Phan et al. [26], who noted that linear models were not performing well compared to ensemble methods when working on complex datasets. While linear regression has its level of interpretability, it is less adaptive in comparison to Random Forest and Gradient Boosting, particularly in highdimensional and nonlinear settings. This work emphasizes the advantages of ensemble models for the prediction of CO₂ emissions in comparison with previous studies using SVM, as stated by Wani et al. [27], and LSTM models, as presented by Kumar and Singh [28]. Support Vector Machines often suffer from difficulties when working with big and diverse datasets, while Long Short-Term Memory networks require substantial computational resources, which limits their use in real-time applications. The following research showcases the fact that ensemble models, such as Random Forest and Gradient Boosting, demonstrate superior forecast accuracy for CO2 emissions. However, Linear Regression remains an important baseline analysis tool. The results support and extend existing studies by providing a scalable framework for future applications in climate policy and energy management.

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