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Review Article
Revolutionizing Antiviral Drug Discovery: The Emerging Role of Artificial Intelligence

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Abstract

Artificial Intelligence (AI) has become a pivotal and transformative force in the search for new antiviral drugs, especially following the COVID-19 pandemic. The pressing demand for effective treatments against new viral threats has underscored the shortcomings of conventional drug discovery methods. The AI, particularly, is revolutionizing the speed at which new antiviral compounds are identified and developed. Incorporating technologies like Machine Learning (ML) and deep learning (DL), AI brings multiple benefits to the drug discovery arena. The AI aids in extensive data analysis and mining, streamlining the identification and filtration of potential drug candidates, thereby reducing the manual effort involved. Another facet of AI, Natural Language Processing (NLP), is instrumental in extracting pertinent information from scientific texts and databases, guiding researchers to relevant drug development data. This automation in information gathering, analysis and interpretation by AI models helps optimize the drug discovery pathway. The effectiveness of AI in antiviral drug development is evident in various instances. Open science projects like the COVID Moonshot have expedited the analysis of thousands of molecules, thus fast-tracking drug discovery efforts against SARS-CoV-2. The AI is also instrumental in repurposing existing drugs for new antiviral uses. The AI models have quickly identified drugs such as remdesivir and hydroxychloroquine as potential COVID-19 treatments, expediting their repurposing. However, AI in drug discovery isn't without its challenges, including data quality, ethical concerns, the need for interdisciplinary collaboration and regulatory hurdles. Ensuring top-notch training data, addressing ethical issues around data privacy and navigating AI regulations are critical to overcoming these challenges. Looking ahead, AI is poised to continue its revolutionary impact on drug discovery by enhancing its speed, accuracy and efficiency. It is anticipated to play a key role in forecasting and preparing for future epidemics and diseases, making it an invaluable asset in combating various health crises beyond antiviral drugs.

Key words: Artificial intelligence, drug discovery, antiviral, deep learning, machine learning

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INTRODUCTION

The onset of the 21st century posed significant challenges globally. The emergence and rapid spread of the COVID-19 pandemic, caused by the SARS-CoV-2 virus, underscored the critical necessity for improved treatment strategies and the development of potent antiviral medications to tackle both new and recurring viral diseases[1,2]. The pandemic underscored the significant danger posed by viral infections, characterized by their swift transmission, elevated death rates and diverse methods of spreading. This led to a worldwide breakdown of healthcare systems and resulted in the deaths of millions. Studies suggest that pandemics similar to SARS-CoV-2 are likely to become more frequent in the coming years, owing to rapid shifts in climate and the effects of globalization[3,4]. However, the only way to combat the threat is through effective antiviral drugs that are rapidly developed and have high efficiency. Effective antiviral drugs are thus essential for treating the viral infection, reducing morbidity and mortality and spread[5].

The recent COVID-19 example has identified many flaws in the current drug discovery, testing, distribution and effectiveness of antiviral drugs. This is demonstrated by the fact that the effective vaccine against the viruses takes almost 15 years and multiple trials to be safe and highly effective[6,7]. Although, the vaccine was developed rapidly during COVID-19, it was less effective as a single dose[8]. Analytical studies suggested multiple vaccine doses or alternate vaccine types are required for optimal efficiency against recent pandemics[9-11].

A significant challenge in developing an effective antiviral control is that, similar to all pharmaceuticals, vaccines too are responded differently by each individual, influenced by their genetic makeup, metabolic processes and environmental factors[12]. Likewise, there is a shortage of appropriate animal models and biomarkers, a complexity in the interaction between the virus and its host and ethical and regulatory challenges in conducting clinical and human trials[13].

Finding antiviral drugs is a complex and challenging task, often less efficient because it depends on multiple sources such as examining current drug libraries and developing new synthetic scaffolds. This complicated nature plays a great role in why producing antivirals continues to be a difficult obstacle in combating diseases like HIV, hepatitis and other similar conditions[14,15]. In this context, Artificial Intelligence (AI) plays a crucial role. It utilizes complex algorithms and artificial neural networks to analyze, understand and develop solutions for complex problems. This review explores the basic concepts of AI, how it functions and its significance in overcoming obstacles in the development of antiviral drugs. As this technology continues to evolve, it presents various ethical and regulatory concerns. The objective of this study provide a comprehensive understanding to clinicians, researchers, policymakers and scientists, assisting them in grasping the essential aspects and the enduring benefits of this technology for humankind.

OUTLINE OF AI

In the AI world, ML and DL are the most important terms used interchangeably. However, both the terms repressed different levels of sophistication. The AI is the overall use of computer learning and abilities for tasks that were previously only considered to be high-level cognitive functions[16]. However, the AI is subdivided into layers, representing the area's complexity. For example, in the AI domain, ML is a system of complex layers processing information through logic. With each layer, the complexity of the information increases and the outcome is an answer comparable to human intelligence. For ML to work, the program has to be trained by humans and the outcomes are moderate for more complex problems. However, for DL, the system is much more complex and independent and behaves like neurons. It grows as the information is processed, learns from its outcomes and answers and has better cognitive and emotional responses[17,18].

In Figure 1, AI demonstrates the technologies deployed in antiviral drug discovery. The ML algorithms are allowing computers to learn from data without being explicitly programmed. These algorithms are crucial for pattern recognition and decision-making based on large datasets. They can be used to identify potential drug candidates by analyzing chemical structures and biological activity data. Decision trees classify data into branches to make predictions, random forests use multiple decision trees to improve accuracy and support vector machines classify data by finding the optimal hyperplane that separates different classes. The DL is a type of ML algorithm modeled resembling the structure and function of the human brain. They are helpful in identifying complex patterns in data and making more accurate predictions compared to traditional ML algorithms. The DL involves neural networks with many layers (hence 'deep') that can learn complex patterns in large amounts of data. These are particularly useful in drug discovery for tasks such as predicting molecular activity, drug-target interaction and generating new molecular structures[19,20]. The NLP technologies can extract information and insights from

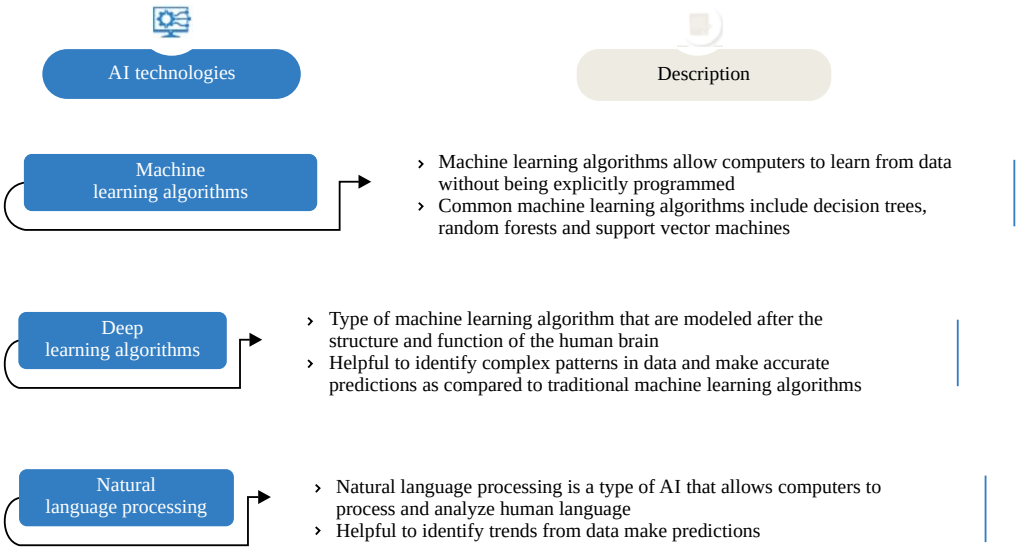

Fig. 1: Overview of AI technologies in antiviral drug discovery
Source: Adapted from Slideteam templates licensed to the corresponding author

scientific literature, patents and clinical trial databases. They can help in understanding the mechanism of viral replication, host response and identifying novel therapeutic targets by processing vast amounts of text data. Advanced NLP models can also assist in sentiment analysis and trend detection within research publications and social media, providing insights into drug efficacy and public health impact[21,22].

The Fig. 1 illustrates the hierarchy and types of AI technologies that are commonly utilized in the field of antiviral drug discovery.

Structure model predictions and compounds generation: Employing a sophisticated AI system in antiviral drug development represents an innovative strategy that shows potential for improving research outcomes. Understanding the structure of viral proteins is a critical element in this endeavor, as it is essential for understanding how viruses trigger infections. This structure is also a central target for many antiviral drugs[23]. Nonetheless, to pinpoint a viable drug target, the virus must undergo testing to determine its potential motif. This process involves conducting numerous experiments, which can be quite time-consuming. The AI, through ML or DL, can expedite this process by predicting the three-dimensional structures of viral proteins based on their amino acid sequences. It utilizes various attributes such as physicochemical properties, evolutionary data and interactions between residues, significantly reducing the time required. This acceleration is primarily due to the elimination or substantial shortening of the most time-intensive experimental phase[24].

The AI in data mining and comprehensive data analysis plays a crucial role in discovering new drug candidates and decoding viral behaviour. Through data mining and in-depth data analysis, we can sift through, categorize and prioritize antiviral compounds, whether they are pre-existing or sourced from natural resources[25]. This process significantly cuts down the time humans would need to identify these compounds. If a drug for a specific virus remains undiscovered despite understanding the virus's 3D protein structure, AI can assist in creating unique artificial molecules to target the virus, with the aid of big data and existing research. Several previous antiviral research investigated thousands or millions of compounds[26-31]. Future developments must then include upgrading the strategy to get benefit from the AI-enforced compounds prediction and analysis systems.

Figure 2 demonstrated that how AI technologies like ML, DL and NLP are revolutionizing the traditional antiviral drug discovery process. It highlights AI's transformative roles across various stages: Target identification, where AI processes vast datasets to pinpoint critical viral components for drug targeting; compounds library screening, which sees AI swiftly predicting potential compounds for target binding; lead optimization, where AI refines the chemical structure of promising compounds; ADMET assessment, involving AI's predictions on a compound's safety and effectiveness and clinical trials, where AI enhances trial design and real-time

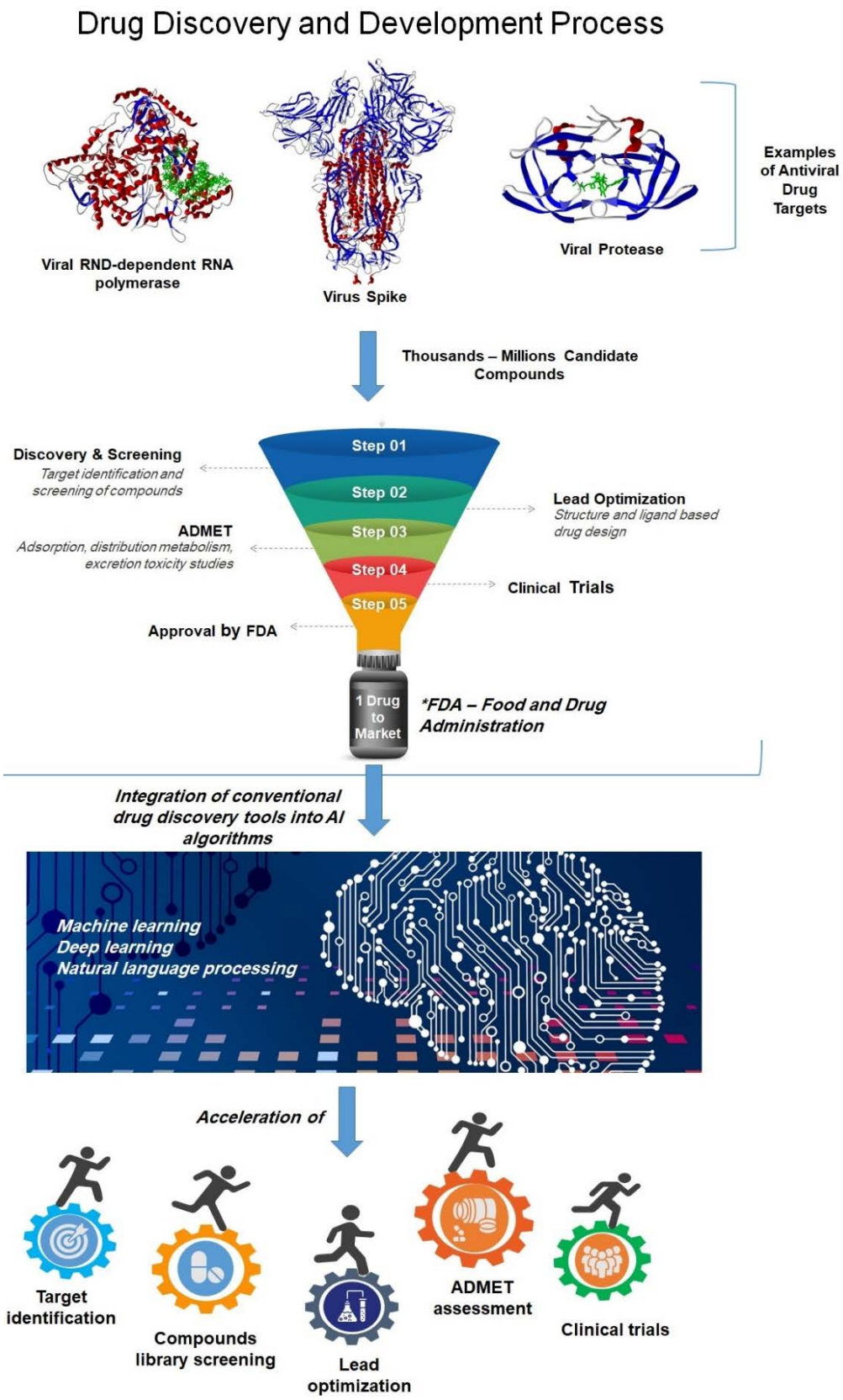

Fig. 2: Role of AI in accelerating antiviral drug discovery

data analysis for quicker efficacy and adverse effect detection. By expediting these stages, AI significantly cuts down the time and cost of developing new antiviral drugs, a boon in urgent outbreak scenarios. This integration of AI into drug discovery signifies a shift towards more efficient, effective approaches in identifying, screening and developing new therapeutic agents.

The viral proteins 3D structures were obtained from the protein data bank accession numbers 7b3d, 6zgg and 3s43 for the viral RNA-dependent RNA polymerase, viral spike and viral protease, respectively. The other content of the image was produced by using SlideTeam templates licensed to the corresponding author.

Leveraging AI to unravel viral mechanics: One of the main hurdles hampering the classic antiviral drug discovery is the need for an accurate virus infection mechanism. Researchers either use *in vitro* experiments or animal models to identify the mechanism of the virus entry, replication and budding, all of which are important in determining the drug effectiveness[27,31,32]. The AI can help us understand these factors by taking into account the data from genomic, proteomic, transcriptomic, metabolomic and phenotypic data. This can help us understand the molecular and cellular processes involved in the viral life cycle and host response. This, in turn, can help us identify the critical stages of the virus infection cycle where it can be better targeted with either the existing drugs or synthetic molecules modelled and predicted by AI[33].

Scientific exploration and NLP for advanced data analysis: Another area where AI is taking the lead and will improve in the future is NLP, defined as the branch of AI that generates human-like speech and written expression. Human language is complex and there are patterns that are associated with each type of language framework[34]. For example, scientific language and literature differ from typical human writing and data. The critical difference is the information's sensitivity, importance and relevance between different literature sections. Scientific literature is a complex yet cohesive written piece that conveys information. The NPC can help us better understand the scientific data from clinical records that otherwise are time-consuming. The NPC can help us extract specific antiviral data extraction, process scientific resources such as PubMed and Google Scholar and identify the information relevant to drug development[35]. For example, using modern AI methods, a scientist or researcher can identify specific and targeted information from millions of papers that otherwise would have been impossible.

The NPC thus can help the scientific community retrieve information with specific queries and extraction as well. Since AI is independent, its use will have the advantage of automation[36]. Nonetheless, the primary benefit is in the evaluation of the gathered data. A proficiently trained AI system, whether it is based on ML or DL, can enhance the process of analyzing this information. Given that numerous factors are considered in drug discovery and the sheer volume of information presents a major challenge for humans, an NLP system can streamline this process effectively[37]. The overall benefit of using AI is thus streamlining the whole process, bringing the time required for identifying the virus mechanism of action, molecular analysis, physicochemical features and identifying targets, thus speeding up the new antiviral drug discovery.

AI and drug discovery collaboration: The AI is not a far-fetched idea for antiviral drug discovery, but it has started to take the shape of reality. The integration of AI in drug discovery is transforming the pharmaceutical industry, promising faster, more efficient and potentially more effective drug development processes. This technological advancement is attracting significant investments and partnerships, indicating a strong belief in the potential of AI to revolutionize the discovery of new drugs[38].

The MoLFormer, a substantial chemical language model created by IBM, specializes in deducing molecular structures from basic formats like the SMILES notation, which outlines the configuration of small organic compounds. Trained on an extensive database of over 1.1 billion molecules, MoLFormer excels in identifying structural patterns and making wide-ranging predictions[39]. It employs an effective linear attention mechanism along with relative positional embeddings. In various fields, including quantum chemistry, physiology and biophysics, MoLFormer has demonstrated superior or comparable results compared to other models. The MoLFormer family is designed to hasten new drug discoveries and assist in designing molecules for diverse purposes, ranging from combating new diseases to developing renewable energy sources[40].

Ongoing research and trials such as the COVID Moonshot are global open science initiatives that use AI and DL mechanisms to design, test and improve potential antiviral drugs for SARS-CoV-2[41]. The project has analyzed over 18,000 new compounds designs and 2400 generated compounds[42]. For researchers, this has revolutionized the whole field of molecular biology and virology as the potential target spectrum has increased many folds and the speed of drug discovery is also unimaginable for the classical antiviral drug discovery system[43].

Recent advancements in antiviral drug discovery: As mentioned earlier, the antiviral drug discovery process is a time-consuming and lengthy process that requires multiple layers of experimentation, predictions and the screening of preclinical and clinical data from other drugs. This, if performed by humans, is a time-consuming process and it can take up to 15 years for a drug to be available on the market. However, situations like the SARS-CoV-2 and related pandemic scenarios require readiness and rapid drug development to save millions of lives. This is where the AI models are indispensable. Their main advantage is the speed and the low margin of error, which is effective and crucial in antiviral deterrence.

Startups and consortiums are becoming increasingly central to the development of fast and advanced viral detection methods. The DIAMONDS (diagnosis and management of infectious and inflammatory diseases by personalised molecular signatures) consortium, led by Imperial College London, is a prime example. It is working on a groundbreaking, multi-disease diagnostic approach using machine learning. The DIAMONDS, is designed to demonstrate that multiple infectious and inflammatory diseases can be diagnosed concurrently through concise gene signatures. Additionally, DIAMONDS seeks to establish a novel categorization of diseases based on RNA molecular signatures and to introduce personalized molecular signature-based disease diagnosis into clinical practice[44]. A beneficial aspect of DIAMONDS is its application to differentiate between bacterial and viral infections by employing biomarkers identified through transcriptomic and proteomic analyses and ascertain the most effective management approaches. A study in Nature introduced the novel concept of using ferrobotics swarms in automated viral testing. This approach is set to significantly boost testing capabilities while reducing costs[45]. These examples highlight the vital role of startups and consortiums in advancing rapid viral screening technologies, crucial for effective disease diagnosis and management.

A comprehensive framework named CogMol has been developed to create new molecules with drug-like properties, aimed specifically at new viral proteins, with a focus on SARS-CoV-2. A deep generative model was used to discover new inhibitors for drug-target proteins without prior knowledge of the target's structure or active compounds. The model was trained on protein sequences and small molecules interactions and utilized protein sequence-dependent sampling. This system integrates the pre-training of a SMILES Variational Autoencoder (VAE) with a controlled method for generating optimal drug-like molecules. The CogMol employs a binding affinity predictor that is trained using SMILES VAE embeddings along with protein sequence embeddings. This framework was used on three target proteins of SARS-CoV-2, leading to the discovery of novel molecules. Additionally, CogMol includes processes for assessing toxicity, the synthetic feasibility and the binding to target structures using docking simulations. The results indicate a high potential for molecules with strong binding affinity[46]. In addition, this model was experimentally tested with proved efficacy. The most potent inhibitor against the spike RBD showed effectiveness against various virus strains in live virus neutralization tests. This approach demonstrates the efficiency of a single adaptable generative model in accelerating inhibitor discovery even when specific target structures or known active compounds are lacking[46].

AI role in antiviral drugs repurposing: New collaborative research groups and data repositories have led to the identification of potential treatments for viral illnesses such as COVID-19, HIV and hepatitis. A notable instance is remdesivir, which was initially created as a general antiviral medication but later repurposed for use against COVID-19[47]. The repurposing of remdesivir was based on clinical trials results supported with hundreds of computational studies. More evidence were collected through virtual screening of the drug using DL models to authenticate the drug effectiveness. The AI-based research determined that remdesivir has an affinity for SARS-CoV-2, which makes it an effective deterrent[48]. Table 1 presented a compilation of drugs that were originally developed for certain diseases but have been repurposed for other medical applications. This repurposing has been identified through the use of advanced AI/ML models, analysis of extensive medical and scientific literature or other conventional tools. Table 1 showcases the original and new uses of these drugs, highlighting the innovative applications discovered through AI-driven research.

A new method called "rapid meta-analysis" (RMA) has been developed, AI to swiftly address clinical questions in times of crisis. The aim was to determine if RMA could offer significant clinical conclusions more quickly than conventional meta-analysis techniques. This approach was tested by investigating the potential ocular toxicity and vision impairment associated with hydroxychloroquine therapy, a drug of particular interest during the COVID-19 pandemic. The combination of AI with human evaluation revealed that RMA could produce a valuable clinical outcome in less than 30 min, calculating an estimated ocular toxicity incidence of 3.4%, though the results varied significantly across different studies. This finding underscores the efficiency of AI-enhanced

Table 1: Overview of various drugs, their primary applications, mechanisms of action, previous uses against specific viruses and corresponding references

Drug	Application	Mechanism of action	Previous uses against disease/virus	References
Nitazoxanide	Antiviral	Broad-spectrum antiviral activity against a range of viruses including coronaviruses	Antiprotozoal agent	Bharti *et al.*[54]
Niclosamide	Antiviral	Broad-spectrum antiviral activity inhibits SARS-CoV replication. It interacts with 16 different proteins	Treatment for tapeworm infections	Rao *et al.*[52]
Chloroquine	Antimalarial potential antiviral	Inhibits viral entry and replication	Treatment for malaria	Eftekhari *et al.*[55]
Remdesivir	Antiviral	Inhibits viral RNA polymerase	Investigational drug for Ebola	Blasiak *et al.*[56]
Ribavirin	Antiviral	Inhibits viral RNA synthesis	Treatment for hepatitis C and RSV	Pires[57]
Favipiravir	Antiviral	Inhibits viral RNA polymerase	Investigational drug for influenza	Ohno *et al.*[58]
Lopinavir	Antiretroviral	Inhibits viral protease	Treatment for HIV	Mohanty *et al.*[59]

meta-analysis in providing quick clinical insights, a notable advancement over traditional methods[49].

Using Optum Life Sciences Claims Data, researchers created Real World Data groups that included more than 3 million patients. They used this data to mimic a clinical trial's observational study structure, aiming to assess the potential repurposing of over 200 FDA-approved medications for COVID-19 treatment. Remarkably, some combinations of these drugs showed effectiveness similar to COVID-19 vaccines. Among the most effective drugs identified was nitazoxanide[50]. Nitazoxanide was deployed in treating giardiasis and cryptosporidiosis. Scientists have used AL/DL models to formulate the optimal drug concentration for the patients. *In silico* and *in vitro* studies supported the application in treating COVID-19[51]. The drug has shown promising results in reducing viral replication in clinical trials, an accurate mechanism yet to be explored[51,52].

The process of discovering small molecule drugs typically involves screening a large number of compounds and then refining the most promising ones through laboratory and *in vivo* studies. Regrettably, approximately 90% of these candidates are unsuccessful in clinical trials, often due to adverse side effects or lack of efficacy[52]. It is suggested that each small molecule drug interacts with about 6 to 11 different targets. This multiplicity of interactions opens opportunities for repurposing existing drugs based on their unintended target interactions. A novel repurposing strategy has been formulated using a combination of AI and predictions based on chemical similarity. This approach examined a dataset of 2766 drugs approved by the FDA and uncovered 27371 off-target interactions involving 2013 different protein targets, averaging about 10 interactions per drug[53]. The drugs most frequently involved in these interactions were those affecting G protein-coupled receptors, enzymes and kinases. Impressively, laboratory validations confirmed 63% of these off-target interactions, many of which were highly effective at low doses. Among these drugs a set of known antiviral drugs or repurposed drugs for antiviral use as remdesivir, telbivudine and niclosamide[52].

The pairing between the repurposed drugs and AI was extended beyond the classical screening followed by antiviral studies. Chloroquine, known for its use in treating malaria and Coronavirus, was chosen as the active pharmaceutical ingredient in solubility studies owing to its repurposing for treating COVID-19. The study focused on understanding its solubility in condensed solvents. The research employed a neural-based modeling method, an approach grounded in AI, to predict the solubility of drugs in these solvents. The model's effectiveness was validated by comparing its predictions with experimental data[53].

Solving uncertain outcomes of antiviral research: Owing to the sudden nature of COVID-19, the pace of antiviral research was increased with lot of contradicting or uncertain outcomes. The IDentif.AI, a platform combining AI and experimental validation, to find effective drug combinations for treating SARS-CoV-2[56]. The researchers tested a 12-drug candidate therapy set against the virus and identified the optimal combination as remdesivir, ritonavir and lopinavir, which was 6.5 times more effective than remdesivir alone. In addition, hydroxychloroquine and azithromycin were relatively ineffective. The IDentif.AI utilized unpredictable drug interactions to identify previously unanticipated, high-ranking drug combinations. The rankings generated by IDentif.AI were consistent with well-documented clinical trial results, even without access to the trial data. This approach reduced testing time significantly and matched clinical trial outcomes, suggesting its potential usefulness in managing current and future outbreaks[56].

Integration challenges: Undoubtedly, speed will be the first advantage of AI-based methods of antiviral drug discovery systems. However, the main hurdle in widespread use will be data quality and how the models were trained for such a sensitive task[60]. We have already determined that ML and DL models need human intervention and data to track, predict and learn, which means the better the quality of the input data for training will be, the better the field results will be.

This poses a significant challenge as AI models still lack sensitivity to the input data, which also leads to ethical problems. For example, what will happen if the data is not appropriately screened, has flaws or human errors are fed to the models? This will lead to the same mistakes humans make, rendering the AI model ineffective for developing antiviral drugs. Parameters like error and biases, heterogeneity and variability, complexity and diversity and dynamism and evolution are the critical data quality parameters[61].

Another challenge is the interdisciplinary nature of the AI in antiviral drug discovery. The virology, computer sciences and ML disciplines are two extreme edges of science. Conforming them into one place is also a challenge that may pose problems when using AI. As a virologist has different training and aims while researching antiviral drugs, computer scientists have different visions. The main challenge will then be to bring the two different disciplines and work on a model that seamlessly binds the two disciplines together. One solution to such a problem is the collaboration mechanisms that can help address the challenges and limitations of AI, such as data quality, algorithm bias and streamlining of data[62].

Similarly, another concern that has alarmed and brought the main hurdle is the regulatory status of such a radical technology shift. The main hurdles in this domain are data privacy laws, algorithm fairness and accountability, human and AI interaction and regulating how much humans can change and influence an AI model[62,63].

Of these situations, data privacy remains the number one concern. Since AI models are trained on actual clinical data of humans with their conditions and diseases, exploiting such sensitive data is one of the main hurdles in popularising the technology[64]. If there are no regulations in place, the AI will have unabated access to sensitive information such as genetic, medical, demographic and gender-based data, which, if caught in the wrong hands, will pose a significant threat to privacy. One way to address this issue is by processing data prior to AI model manipulation and training. Similarly, algorithm fairness and accountability are also a concern among scientists who consider the decisions made by AI models to have an accountability mechanism.

Future perspectives: The AI has become indispensable part of medicine and healthcare and this is just the beginning. It will play an essential role in the antiviral drug discovery process. It can help overcome challenges and limitations that slow down the classical drug discovery mechanism, such as cost, time and accuracy. The AI can also enable us to explore new opportunities and possibilities, such as more effective and entirely artificial drugs that have low toxicity, higher success rate and effectiveness[65]. In the future, this will be even more sophisticated as the models will evolve and better DL methods will be available for data processing.

The use of such a sensitive and powerful tool is not just limited to antiviral drug discovery but also has the potential to play an important role in predicting future epidemics and disease outbreaks based on the current scientific data. The same models can also then predict the vital aspects of such a pandemic, such as mortality rate, novel targets for drugs and ultimately artificial drugs based on the predicted data[66]. For example, BlueDot, a Canadian AI company, predicted the SARS-CoV-2 outbreak in China before its announcement by WHO[67]. This shows the power of AI systems to prepare the world for challenging scenarios.

CONCLUSION

The AI models are becoming crucial in antiviral drug discovery and the pharmaceutical industry due to their superior data handling, prediction-making and drug discovery capabilities compared to traditional methods. Traditional approaches are slow, costly and less successful, making them ill-suited for addressing pandemics like COVID-19. The AI promises to improve personalized medicine, enhance pandemic management and predict virus spread, mortality rates and drug targets accurately. It also enables simulations for drug discovery that classical methods cannot achieve. However, AI technology raises concerns, including ethical issues related to the use of personal data for training models and the lack of effective global legislation to govern AI development. There is a need for comprehensive global regulations to address bias, algorithm unpredictability, accountability and transparency in AI.

SIGNIFICANCE STATEMENT

This review highlights the transformative role of Artificial Intelligence (AI) in advancing antiviral drug discovery post-COVID-19 epidemic. The AI, through Machine Learning (ML), deep learning (DL) and Natural Language Processing (NLP), enhances the efficiency, speed and accuracy of identifying new antiviral compounds, significantly reducing manual efforts and expediting drug development. Key findings underscore AI's success in rapidly screening and repurposing drugs. These advancements are critical as they offer a promising avenue to overcome the challenges in drug discovery, suggesting further exploration into AI's potential to predict and prepare for future health crises and viral epidemics, thereby revolutionizing the antivirals landscape.

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