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Artificial Intelligence: A New Trend in Drug Designing Against SARS Cov-2

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Abstract- The Covid-19 manifested its destructive effect all over the world leading to a huge loss to mankind. Therefore, the development of a vaccine against coronavirus was the only way to tackle this pandemic. SARS-CoV-2, the causative agent of the Covid-19 pandemic, consists of around 30 different proteins (some of which are M, E, N, and S proteins) and it was difficult to determine all the structural proteins of the virus for the development of vaccine due to frequent changes in its variants. Conventional methods were not able to predict the target protein precisely in a short period. Therefore, SARS CoV-2 has transformed the outlook of research in pharmacy by encompassing Artificial Intelligence (AI) to predict the accurate structure of a protein. Researchers utilized different AI tools such as Alphafold2, CoVex, VirHostNet, etc. to predict the 3D structure of target protein and ligand affinity to design vaccines against the virus. Hike in the usage of AI techniques was observed after the pandemic since many pharmaceutical companies adapted AI to rapidly design vaccines against coronavirus within a short period and that too with high efficiency and optimal cost. Although AI approaches shorten the duration of drug development from 10-12 years to 1-2 years we need skilled data scientists to operate these tools because it is difficult to understand the algorithm for everybody. AI eases the drug designing process in many ways but researchers cannot completely rely on its results since it has its limitations.

Keywords- Artificial Intelligence, Drug Designing, SARS CoV-2, AI tools.

I. INTRODUCTION

No one is unaware of the devastating situation that the world went through during the pandemic. Covid- 19 caused substantial loss to human life, economy, education, our mental health, and whatnot.

The loss was so dramatic because of the unavailability of proper treatment against SARS-CoV-2. This unavailability led to an incredible amount of pressure on the pharmaceutical industries to develop a vaccine against this deadly virus, which too during a very short period.

Using conventional methods for drug discovery may be a very time-consuming process, so, this was the instant when AI came to the rescue of our scientists. Artificial Intelligence is nothing but programming computer systems in such a way that they can perform tasks that normally require human intelligence. Some of the AI tools like AlphaFold2, VirHostNet, etc. played a major role in the drug discovery process by predicting the 3D structure of various proteins present in the Corona Virus.

There are about 30 different proteins present in the structure of SARS CoV-2 that can be studied with the help of AI, some of which are,

1. **Spike (S) protein:**
Present on the surface of the virus and are responsible for the attachment of SARS CoV-2 to the ACE 2 receptors

2. Nucleocapsid (N) protein:
Present in the matrix and is bound to the ssRNA.

3. Envelope (E) protein and Membrane (M) protein:
Together they make the envelope of the virus.

Scientists were able to study all these proteins in detail because of different AI tools. Not only in drug designing but AI also played an important role in reporting adverse drug reactions and identifying patients for clinical trials. The role of AI in drug designing can be classified into three main categories

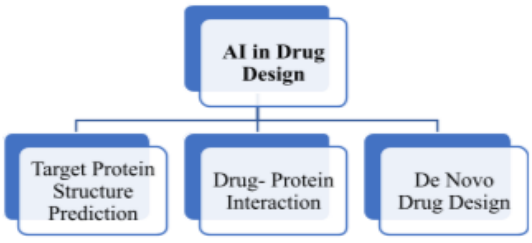

Fig 1. Role of AI in Drug Designing.

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4. Target Protein Structure Prediction:
Prediction of the Target Protein is one of the most crucial steps towards drug designing. We need to predict the structure of the target protein so that selective targeting of disease can be done. AI tools can be efficacious in estimating the 3D structure of the desired protein.

5. Drug- Protein Interaction:
Drug- Protein interactions are crucial to understanding the efficacy of the drug. Various AI tools can predict these interactions precisely. This ability of AI was also proved to be useful in assisting the repurposing of existing drugs. Repurposing an existing drug not only qualifies it directly for the Phase 2 trials but also reduces the expenditure.

6. De Novo Drug Design:
"De Novo" means from the beginning i.e., designing a drug molecule without any starting template. AI is replacing the traditional methods of de novo drug designing because of shortcomings of complicated synthesis routes and difficult prediction of the biological activity of the novel molecules. With the help of Computer-aided drug designing (CADD), it is possible to predict millions of structures that can be synthesized.

II. VARIOUS AI TOOLS USED IN DRUG DESIGNING AGAINST SARS COV-2

Artificial Intelligence played the most pivotal role in drug designing against SARS CoV-2. AI tools proved to be very useful in determining the 3D structure of various proteins present in SARS CoV-2, viral and host protein-protein interactions, and repurposing of many drugs.

Repurposing of drugs means using the already existing drug for some other purpose (disease). For example, antimalarial drug hydroxychloroquine was repurposed and was found to be useful in many Covid patients.

Table 1 and Table 2 are depicting the use of AI tools in drug design and AI models in repurposing drugs against COVID-19 respectively.

Table 1. AI tools and their role in drug designing.

S.no	AI Tool	Manufacturer	Function
1.	AlphaFold2	DeepMind	Predicts the 3D structure of target protein by calculating the distance between the adjacent amino acids and the corresponding angle of the peptide bond.
2.	VirHostNet	Elixir bio.tools European Virus Bioinformatics Centre FAIRsharing.org	It is a fair and open data resource that contains data about various protein-protein interactions (between SARS CoV-2 and host cellular protein).
3.	P-HIPSTer		Database for information about virus-host protein-protein interactions (PPIs) further helps in studying molecular interactions leading to viral infection and determining host factors and pathways that may act as potential drug targets to treat the infection.
4.	CoVex	Biō keanós Elixir bio. tools	Database for integration of virus-host protein interaction, human protein-protein interactions, and drug-target interactions. It was found to be useful in the repurposing of drugs during Covid19.

Table 2. AI tools used in the repurposing of drugs against COVID-19.

1.	Molecular Transfer Drug Target Interaction (MT-DTI)	Remdesivir, Efavirenz, Ataznavir, Dolutegravir	They have inhibitory potency on 3CL protease; targeting viral proteins of SARS-CoV-2.
2.	Deep Graph Neural	Aspirin, Atorvastatin Albuterol, Azithromycin, Acetaminophen	These drugs showed multiple interactions including host genes, pathways, and virus baits.
3.	Autoencoder -based architecture	Quinapril, Ribavirin, Clemastine	AI is used to learn the gene expression profiles of drugs and the SARS-CoV-2 virus.
4.	Graph Convolutional Network	Tenofovir, Darunavir, Ribavirin,	GCN precisely identified the drugs, effective

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	(GCN)	Lopinavir,	against SARS-CoV-2.
5.	Text Mining	Poly-ADP ribose polymerase 1 inhibitor, CVL218 and Fapilavir	CVL218 and fapilavir inhibit the replication of the virus and prevent the immunopathology caused by a coronavirus.

III. ACCELERATION IN RESEARCH AFTER INTRODUCING ARTIFICIAL INTELLIGENCE

Artificial Intelligence approaches are easier to predict 3D structures of receptors, proteins, and/or enzymes as compared to traditional approaches. This technique can also predict the activity of thousands of unsynthesized compounds and therefore, AI techniques have surpassed all conventional approaches.

AI hastens research in the field of pharmacy due to the following reasons:

- AI provides precise and definitive outcomes, whereas conventional methods include random screening; therefore, it is more likely that the results will be vague.
- Conventional methods take around 10-16 years to design a drug because of blind screening, whereas due to specific and target-based processes AI completes the drug development within 6-8 years.
- As traditional methods are time-consuming, it makes the process more costly, whereas AI costs about one-third in drug development.
- Communication between disciplines and management of the process are well maintained with AI approaches, whereas difficulty in management and irrational communication between disciplines are the drawbacks for the speedy discovery of a compound using traditional approaches.

In the pandemic era, many pharmaceutical companies opted for AI technologies over conventional techniques. AI technologies like IBM's AI identified several small molecules that could bind to the spike protein of SARS-CoV-2 and inhibit interaction with the human angiotensin-converting enzyme (ACE2) receptor. Researchers at USC Viterbi School of Engineering designed an ML model to speed up vaccine analysis and look over mutations in the virus. Iktos' AI has also been adopted by many pharmaceutical companies to predict small molecule activities for de novo design.

These AI models reduced the challenges of traditional drug design by saving time and providing more automation. But along with the advantages, AI also has some drawbacks which should not be neglected.

IV. DRAWBACKS

The biggest limitation of using AI in drug design is the lack of skilled persons to operate AI and understand the algorithms. One must involve data scientists with sound knowledge whenever dealing with AI. Other than the need for skilled people, sometimes even the researchers create algorithm bias to get desired predictions from machine learning. Another challenge researcher's face while using AI is its cost of installation as it takes a significant investment to get installed.

Along with difficulty in understanding the algorithms, it is also hectic to explain the working of AI models and interpretation of its results; therefore, in the end, scientists have to double-check the results on their own.

Another drawback of using AI in drug design is the conversion of conventional preliminary research into a machine language. Because of these challenges, a scientist cannot totally rely on AI technologies but still could be free from all the overburden faced by them.

V. CONCLUSION

AI tools proved to be a strong approach for designing vaccines against the virus, accelerating education and research in pharmacy. It reduces the complications associated with traditional methods and improves the design, delivery, and surveillance of vaccines. It also reduces the use of animal models in preclinical screening and that's why it is found to be a good alternative for animal experimentation.

AI diminishes the burden of data collection and accelerates the research in pharmacy with algorithm accuracy signifying the future utilization of AI tools to develop drugs against untreated diseases or designing new drugs against existing diseases with better pharmacological properties.

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