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Artificial Intelligence Based Drug Discovery Techniques for COVID-19 Detection

Kawal Arora[1], Ankur Singh Bist[2]
Signy Advanced Technologies, India
Address : Level 39, One Canada Square, Canary Wharf, London E14 5AB
e-mail: kawal@signy.io[1], ankur@signy.io[2]

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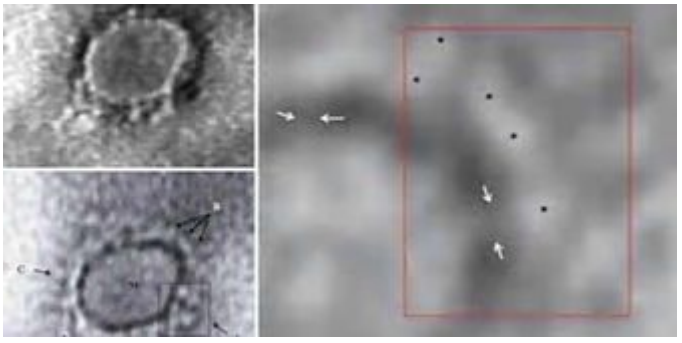
Abstract

Recent advancements in the area of drug discovery using artificial intelligence made it possible to speed up the hunt for new pharmaceuticals. Drugs like arbidol, atazanavir, ramdev sivir & favipiravir are under testing phase to cure COVID-19. In this paper, we present systematic study of AI based drug discovery techniques suitable for COVID-19 detection.

Keywords: Coronavirus, artificial intelligence, drug discovery and drug selection.

1. Introduction

Coronavirus is a specific type of virus and as per inherited property replicates and expands. Seriousness of this virus is due to Its nature of expanding with very fast pace. Picture 1 shows the basic structure of coronavirus. Mammals and birds are attacking points of this virus. This disease cause variety of infections related to respiratory system.



Picture 1: COVID-19 by electron microscope (Indian Council of Medical Research)

Coronavirus origination started from china and expanded in different parts of world. Most of the countries declared it as medical emergency. Till March 2020 around 40000 deaths are confirmed due to this. Picture 2 depicts the coronavirus spread.

Picture 2: Coronavirus spread

Governments developed various isolation centers to take care infected patients. Sanitization procedures are taken at wide scale to mitigate the effect of this epidemic. Picture 3 shows the efforts made by government agencies to tackle the situation.

Picture 3: Coronavirus Prevention

Government efforts are not sufficient to tackle the situation alone. Without efforts of common men it's not possible to control the disaster. Picture 4 shows some common precautions required by everyone in this situation. In case of any symptoms, medical checkup is necessary. Common questions & answers related to COVID-19 are released by WHO: https://www.who.int/news-room/q-a-detail/q-a-coronaviruses.

Advice for common public released by WHO can be found at: https://www.who.int/emergencies/diseases/novel-coronavirus-2019/advice-for-public.

Picture 4: Preventive Measures

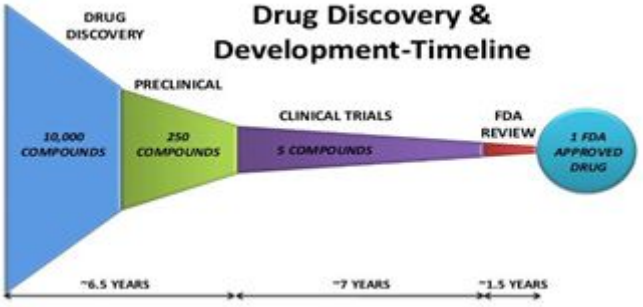
AI can be used to tackle this situation:

1. By analyzing Chest X-Ray, CT-Scans and other clinical symptoms to detect COVID-19
2. By doing drug or vaccine discovery for Covid-19 virus

3. By analyzing the effect of existing medicines on Covid-19 virus
4. By analyzing the remedies for current and future attacks of same type

2. Drug Discovery Based on AI

Drug discovery is the process of finding drug for new diseases. It involves target identification, target validation, lead identification and lead optimization. Identification of protein that has specific function with disease is called target identification. Verification of target as per inventor thought process is called target validation. Process of identifying best compounds with respect to target protein is called lead identification. Lead optimization is the process of ensuring drug associated characteristics of compounds. Inventor has to assure about bioavailability, specificity and toxicity of identified compounds. The process of testing compounds with animals to check the response of compound is called pre-clinical testing. Picture 1 explains the drug discovery and development timeline.



Picture 5: Drug discovery process [1]

COVID-19 is major issue in front of world; continuous process of drug/vaccine discovery is going by various research groups and pharma companies. As per research article [2, 3] antiviral drugs and process of treatment for COVID-19 is mentioned in table1.Still research is going on these drugs and actual medicine is yet to come.

S.No.	Drug	Process of treatment
1	IFN-α	Vapor inhalation, 2 times/day, duration of treatment: maximum 10 days
2	Lopinavir/ritonavir	Oral, 2 times/day, duration of treatment: maximum 10 days
3	Ribavirin	Intravenous infusion, 2-3 times/day, duration of treatment: maximum 10 days
4	Chloroquine phosphate	Oral, 2 times/day, duration of treatment: maximum 10 days
5	Arbidol	Oral, 3 times/day, duration of treatment: maximum 10 days

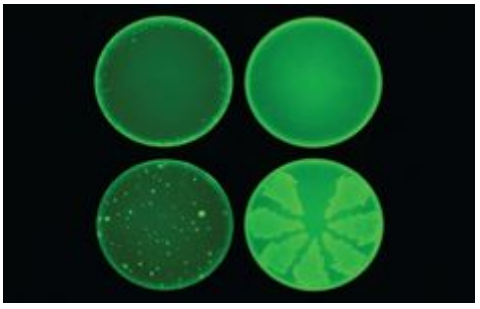
Table1: Treatment Guideline for COVID-19 [2,3]

As per research [3] following agents are found useful against SARS-CoV-2. In January 1996, Merck & Co. found that indinavir was a clinically capable medicine depending on data from human trials. Saquinavir was found by the pharmaceutical company Roche and approved by food and drug administration, US. Similarly other drugs are verified by different agencies and worked well for other medical causes.

1. Indinavir
2. saquinavir
3. lopinavir

4. carfilzomib
5. ritonavir
6. remdesivir
7. atazanavir
8. darunavir
9. tipranavir
10. fosamprenavir
11. Enzaplatovir
12. Presatovir
13. Abacavir
14. Bortezomib
15. Elvitegravir
16. Maribavir
17. Raltegravir
18. Montelukast
19. Deoxyrhapontin
20. Polydatin
21. chalcone
22. disulfiram
23. carmofur
24. shikonin
25. ebselen
26. tideglusib
27. PX- 12
28. TDZD-8
29. cyclosporin A
30. cinanserin
31. Rhizoma Polygoni Cuspidati
32. Radix Sophorae Tonkinensis

AI has been harnessed to develop compounds i.e. chemically correct and useful against new diseases. AI based algorithms can be trained with crucial characteristics of know drug. Trained AI program can organize new molecules based on learning and it will lead to the synthesis of useful compound. AI can be used in searching good compounds, drug targets, chemical modifications etc. Authors in paper [4] used AI techniques to speed up and optimize the drug selection process. MIT researchers used ML algorithm to find drug called halicin [5].



Picture 6: Halicin drug

Authors in paper [6, 7] discussed about Drug targeting and designing using artificial intelligence. AI subfields machine learning; deep learning and reinforcement learning are mainly used for sorting out various issues of healthcare. Let's tag AI subfields with healthcare related tasks under following points.

S.No.	AI Packages	Web links
1	AlphaFold	https://github.com/deepmind/deepmind-research/tree/master/alphafold_casp13
2	DeepChem	https://github.com/deepchem/deepchem
3	MOSES	https://github.com/molecularsets/moses
4	Biopandas	https://github.com/rasbt/biopandas
5	Chemprop	https://github.com/chemprop/chemprop
6	OpenChem	https://github.com/Mariewelt/OpenChem
7	ReLeaSE	https://github.com/isayev/ReLeaSE
8	Neural-fingerprint	https://github.com/HIPS/neural-fingerprint
9	HTMD	https://github.com/Acellera/htmd
10	Gnina	https://github.com/gnina/gnina
11	ChemGAN challenge	https://github.com/mostafachatillon/ChemGAN-challenge
12	DeepNeuralNet- QSAR	https://github. com/Merck/DeepNeuralNet-QSAR
13	NNScore	http://rocce-vm0.ucsd. edu/data/sw/hosted/nnscore/
14	SIEVE-Score	https://github.com/sekijima-lab/SIEVE-Score
15	Hit Dexter	http://hitdexter2.zbh.uni-hamburg.de

Table 2: AI for drug discovery

2.1 Machine Learning

1. Supervised Learning (Disease predication & Drug efficacy)
2. Unsupervised Learning(Evaluating disease subtype & disease target discovery)

2.2 Deep Learning

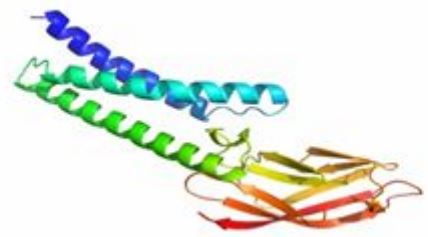
1. To process medical data for disease prediction like CT-Scan, Chest X-Ray etc.

2.3 Deep Learning

1. Drug design decision making
   Researchers believe that the process of drug discovery will be totally changed with the advancements of artificial intelligence.

3. AI Based Tools And Techniques For Drug Discovery

Moderna Therapeutics, a biotech company developed vaccine in context of COVID-19 in less than 2 months after the genetic sequence of the SARS-CoV-2 [7]. Researchers are using AI based technique to find molecule that can halt Coronavirus replication. Table2 contains summary of AI packages that can be used for drug discovery. AlphaFold, DeepChem, MOSES, Biopandas, Chemprop, OpenChem, ReLeaSE, Neural-fingerprint, HTMD, Gnina, ChemGAN challenge, DeepNeuralNet- QSAR, NNScore, SIEVE-Score, Hit Dexter are some AI based tools used for the task related to drug discovery, protein modeling etc. Let's discuss state of art AI systems for drug discovery. AlphaFold [9] is developed by DeepMind for protein folding prediction. AlphaFold pipeline use three different networks. At level1 variable auto-encoder (DRAW) is used to create fragments. At level2 simulated annealing is used to combine fragments then for last step, scoring process takes place with the help of co-evolutionary residues and scoring networks (3D based approach). Combination of protein model and energy model give rise to final protein. Picture 7 shows the protein structure prediction associated to COVID-19.



Picture 7: Protein structure prediction related to COVID-19[10]

DeepChem is open source tool that bring up the use of deep-learning in drug discovery. Drug discovery datasets are very costly and if available cannot be easily used due to ethical reasons. Author in experimental analysis [11] found that one-shot learning integrated with deepchem for drug discovery. Similarly other openly available tools as mentioned in table2 works on different aspect of drug discovery using artificial intelligence. Already various research communities and companies have used power of AI to find out drug suggestions for COVID-19. Clinical trials and approval process of drugs synthesized by AI for COVID-19 is going on. Everyone is hoping to get the outcome in this context as soon as possible.

4. Conclusion And Future Work

In this paper we summarized the current scenario of AI based drug discovery for COVID-19. Understanding protein synthesis, molecular changes, time management in laboratory are some important requirements to accelerate the process of drug discovery. AI/ML/DL techniques will work on each attribute of speedup drug discovery. AI based architectures are evolving with very fast pace, that will be helpful for designing robust system. Current work will be very useful for industrial or academic purpose.

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