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IIIT D develops AI model to repurpose existing drugs for COVID-19 treatment

13 July 2020 | News

The AI model computes the similarity between the chemical structures of the drugs and the similarity between the genomic structures of existing viruses and the novel Coronavirus



In a bid to counter the coronavirus pandemic that has been rampaging around the world,Indraprastha Institute of Information Technology (IIIT) Delhi has worked on computational AI (Artificial Intelligence) model for drug repositioning in the treatment of COVID-19.

This essentially means that instead of manually going through ever available drug and checking its effectiveness against COVID-19 (which is a painstakingly long process), we can now rely on AI to speed things up and find us the drugs which have the highest probability of success against the disease.

The AI model that could prove to be an indispensable tool in the battle against COVID-19 has been the result of collaboration between Indraprastha Institute of Information Technology (IIIT) Delhi, IPGME&R Kolkata and INRIA, Saclay, Paris, France.

The database of drugs (drugbank.ca) lists more than 100 approved antivirals. Trying out all of them in clinical trials is not possible; it will be expensive both financially and in terms of time – a luxury we cannot afford. Therefore, AI can be used to prune this massive database and select a handful (5 to 10) of drugs that have better chances of succeeding. This would allow more concerted effort/trials on this handful of prospective treatment regimes.

To find out the best possible treatments for COVID-19, IIIT- Delhi follow the approach of drug target interaction (DTI) prediction. This is a standard approach in computational drug repositioning, i.e. reusing a drug that was developed for a certain disease for treating a different ailment. One classic example is Imatinibmesylate (sold under the trade name Gleevec) which was originally developed as a treatment for leukemia, and was later repositioned to treat gastrointestinal stromal tumors.

In simple terms, the AI model computes the similarity between the chemical structures of the drugs and the similarity between the genomic structures of existing viruses and the novel Coronavirus. The model then looks at the historical information about the efficacy of the drugs on different viruses; it selects similar drugs (based on chemical structure) that have been successful in treating viruses that have a genomic structure close to that of the novel Coronavirus.

Thus far, the AI models have selected Remdesivir, Umifenovir, Ribavirin and Sofosbuvir as prospective cures, and all of them are undergoing trials for COVID-19. The computational model and the state of clinical practice are thus in sync with each other.