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Drug Repurposing as a Weapon to Combat Covid-19 Pandemic: The *In-Silico* Drug Design Approach

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Abstract

Drug repurposing, also known as drug repositioning or drug reprofiling, involves the establishment of new medical uses for already known drugs, including approved, discontinued, shelved and experimental drugs. While with standard Drug Discovery path an investigational molecule may take 10 to 15 years to come to the market (by going through different stages starting from understanding disease followed by target identification, assay development, High Throughput Screening, Lead identification, pre-clinical trials, FDA approval, clinical trials and finally introduction to the market after FDA review), drug repurposing may reduce the time to 2 to 5 years by bypassing the steps of pre-clinical and clinical trials and FDA formalities as the drug is already in use for some other disease. Although this strategy has been known since long, it has gained considerable momentum in the current scenario of COVID-19 pandemic where a quick solution is needed to combat the disease as we enter a phase beyond containment. For targeting SARS COV-2 proteins with drugs, the Non Structural Proteins (NSP) which include Replication Complex (NSP6), SS RNA Binding (NSP9), Helicase (NSP13), 3'-5' exonuclease (NSP14), Protease (NSP5) and RNA dependent RNA Polymerase (NSP12) have been identified. As the later two targets are specific to SARS COV-2, inhibition of these would not affect the human cells and be specifically effective against the virus. Ritonavir/ Lopinavir that inhibit protease and Ramdasivir which inhibits RNA dependent RNA Polymerase are the drugs that are being used in some cases. The problem is, these drugs are so expensive and a more effective alternate is urgently required; Computational or *in-silico* approach towards finding the new alternative is the solution. From a library of about 1.2 million compounds active against SARS COV-2 NSP-12, one can identify the best lead molecule though computational studies and after virtual screening and observing clinical effects, the better may come to the clinic via the shortest route.

Keywords: Drug Repurposing, COVID-19, SARS COV-2 proteins, RNA dependent RNA Polymerase, In-Silico drug Design.

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