Bioinformatics Research Group at UMT Identifies Naturally Occurring Compounds Having Anti-Viral Effect for Treatment of COVID-19 using AI based Simulations

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Description:

RNA-dependent-RNA polymerase (RdRp) protein is a key enzyme used by any RNA virus. It replicates the virus using viral RNA when it enters into the human cell. It creates viral genomes inside the human body. Once the virus gains entry into a cell it uses the cell resources to replicate itself making the cell sick and leading to its eventual death. The replication of the virus is the main process that acts as a catalyst in the progression of disease in a COVID-19 patient. Key binding sites of RdRp Protein are ASP 618, ASP 623, ASP 760, ASP 761, ASN 691, SER 682, THR 680, ARG 555, and VAL 557. A drug therapy that targets these residues of RdRp protein will be able to produce an antiviral effect by inhibiting its function. Moreover, clinically proven drugs like Remdesivir binds to THR 680, SER 682, and VAL 557 and pp-sofosbuvir binds to ASN 691, ARG 555, and ASP 623. To stop the replication, most suitable natural antiviral compounds are suggested that can play vital role. These naturally occurring compounds bind with the key residues of RdRp protein that are main cause of replication. Following are the compounds that bind to key sites and inhibit the mechanism of virus.

1. Quinic acid (multiply acylated with galloyl moieties) (PubChem ID: 442676) (Represented in Blue)
2. 5-Amino-2-(4-amino-3-fluorophenyl)-6, 8-difluoro-7-[hydroxy-(3-hydroxypropylamino) methyl] chromen-4-one (PubChem ID: 67771200,) (Represented in Orange)
3. Sennaglucosides (PubChem ID: 5199) (Represented in Magenta)

These compounds can be used simultaneously in combination to stop the replication of virus from spreading inside the host cells. The most promising observation from the simulation is that a therapy based on the combination of above described compounds can bind to eight out of nine key residue sites of RdRp protein of Sars-Cov-2 with good binding affinity. The binding key sites which these compounds cover, are ARG 555, THR 680, SER 682, ASN 691, ASP 618, ASP 623, ASP 760, and ASP 761. This combination will surely help to stop the replication of virus by covering the catalytic sites of RdRp. Below is illustration of Potential compounds binding with key sites of RdRp.