In-silico Prediction of Desoxyhavannahine as a Potential Novel Inhibitor of SARS-COV-2 with Minimal Side Effects

Abujamil, Lana (School: Manarat Al-Madinah National School)

Severe acute respiratory syndrome (SARS-CoV-2), has caused the global infectious disease COVID-19. Cases of COVID-19 infections increased rapidly along with high mortality rates and therefore efficient medications are needed. Researchers have turned to antiviral drugs and several show promising results but also bear negative side effects. This study uses computer software to determine if desoxyhavannahine, an antibiotic compound found in Red Sea soft coral, possesses anti-viral activity against crucial proteins that contribute to the replication and entry of the virus. These include RNA dependent RNA polymerase (RdRp), spike glycoprotein, and Papain-like protease (PLpro). The protein structures were obtained from the RCSB protein data bank and the compound structure was obtained from the PubChem database. The compound's efficiency to inhibit active sites, consequently preventing the virus from functioning properly, is determined by low binding energy measured using docking servers. The lowest binding energy was achieved when binding to PLpro with a score of -8.5 kcal/mol. Molecular dynamics software was used on RdRp to evaluate the binding in a realistic manner. The results showed the root mean square deviation values of the protein and compound were considerably low, ranging between 1-3A, indicating the stability of the docking throughout most of the simulation. The compound's drug-likeness and toxicity were evaluated using absorption, distribution, metabolism, and excretion (ADME) profiling software. The predicted results showed that the compound can be easily distributed and is low in toxicity. These outcomes suggest that desoxyhavannahine, a potential inhibitor, is a candidate for further tests in wet labs.

Awards Won:

Fourth Award of $500