Analyzing the Efficacies of Potential Inhibitors of Drug Targets Human Receptor ACE2 and Viral Replication Enzyme RdRp Against SARS-CoV-2

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SARS-CoV-2 is the virus behind the Coronavirus pandemic, contributing to over one million deaths and forty million infections. Forms of COVID-19 prevention are of immediate concern. This study sought to identify inhibitors of drug targets ACE2 and RdRp through molecular docking studies to find a method to minimize the spread of SARS-CoV-2. The inhibition of drug targets ACE2 and RdRp was studied through the docking of ten ligands using Autodock Tools, VINA, and PyMOL. For ACE2, the best-binding ligand was ivermectin (-18.4 kcal/mol). All ligands were stronger than the control, NAG (-6.3 kcal/mol), found in the crystal structure of the bound protein. For RdRp, GTP produced the most negative binding free energy of -11.0 kcal/mol. The control (remdesivir, chosen for its current use as medication for COVID-19) had a binding energy of -9.1 kcal/mol. Thus, ACE2 binds more favorably to the proposed ligands than RdRp; however, further research on in vivo complications will be necessary before definitively identifying the more suitable drug target. Ultimately, this data supports the hypothesis that these ligands can become potential inhibitors of the drug targets of SARS-CoV-2 based on binding favorability: A more negative binding energy indicates a more stable protein-ligand complex, and thus a more effective inhibitor, since the reaction of bonding resulted in lower-energy products. This study opens up the possibility of developing inhibitors of SARS-CoV-2. However, binding value alone cannot be used to determine the viability of these drugs as medication — in vivo complications must be taken into account. Nonetheless, while the binding energies may not directly correlate to effectiveness in inhibiting SARS-CoV-2, they provide a starting point for further research.

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