ABSTRACT

In Silico Screening of Antiviral Compounds from Natural Product Against Corona Virus (COVID-19)

Honey Dzikri Marhaeny

Coronavirus outbreak is a global health crisis that occurs almost throughout the world. In order to COVID-19 drug discovery, chalepin, phyllanthin, hypophyllanthin, rutin, arborinin, curcumin, and quercetin are selected as potential compounds against COVID-19 main protease (6LU7 and 5R7Y) through the receptor-ligand interaction on its pharmacophore. These isolate compounds have been reported to combat several RNA viruses. Based on literature, aromatic ring structure, –OH, –C=O, and $–OCH_3$ groups gave an important role in antiviral protein-ligand bonding activity. This study uses Molegro Virtual Docker 6.0 to determine the best binding energy through the rerank score which shows the total energy bonds calculation. The rerank score of those compounds will be compared by its native ligand of receptor where the lowest energies indicate a strong and stable bond against receptor. The rule of five (RO5) by Lipinski is also used to evaluate the drug-likeness of ligands.The results showed rutin violates three criteria of RO5 because its categorized as beyond of RO5. The docking analysis showed rutin which gives the lower rerank score than inhibitor N3. Meanwhile, several compounds except arborinin gave the lower rerank score than Z45617795. Furthermore, the hydrophobicity and electrostatic interactions also observed. Rutin showed the best interaction if it compared to other compounds. In conclusion, rutin predicted to have strong activity against COVID-19 instead of 6LU7 native ligand, inhibitor N3. While, chalepin, phyllanthin, hypophyllanthin, rutin, quercetin, and curcumin predicted to have a strong activity against COVID-19 instead of 5R7Y native ligand, Z45617795. Further research is needed to support the discovering of COVID-19 phytotherapy through bioassay studies.

Keywords: antiviral, COVID-19 main protease, docking, in silico, natural products