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Developing potential drugs for COVID-19 using ligand based virtual screening

Background and purpose: Coronavirus disease 2019 (COVID-19) caused by Severe Acute Respiratory Syndrome-Coronavirus 2 (SARS-CoV2) is a highly contagious disease that has infected more than 13 million patients and led to more than 580, 000 deaths in less than seven months. Chloroquine is very effective in management of COVID-19. Compounds similar to chloroquine may have the same biological activity and thus inhibit SARS-CoV2.

Methods: SwissSimilarity tool was used to identify similar compounds to chloroquine in the ZINC database. Compounds which were more similar than hydroxychloroquine were selected and used to test molecular docking with quinone reductase 2 (a target for chloroquine). Pharmacokinetic and toxicity profiles of selected compounds were assessed using SwissADME and Protox Server respectively.

Results: There were 49 drug-like compounds in the ZINC database having a higher similarity index to chloroquine compared to hydroxychloroquine. 17 of these had a better binding potential to quinone reductase 2 compared to chloroquine while two had similar binding potential to chloroquine and three had similar binding potential to hydroxychloroquine. Out of these 22 compounds, 18 had a higher predicted LD50 compared to chloroquine but lower when compared to hydroxychloroquine.

Conclusion: Eighteen drug-like compounds in the ZINC database bind with high affinity to quinone reductase 2, are less toxic but similar to chloroquine. Therefore, they may have activity against SARS-CoV2. However, in vivo or in vitro study should be done since this is an in silico study.

Keywords: COVID-19, SARS-CoV2, chloroquine, quinone reductase, ZINC database, ligand-based virtual screening

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