JOURNAL OF NATURAL REMEDIES
DOI: 10.18311/jnr/2020/25278
RESEARCH ARTICLE

In Silico Screening of Traditional Herbal Medicine Derived Chemical Constituents for Possible Potential Inhibition against SARS-CoV-2

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Abstract

The outbreak of SARS-CoV-2 has initiated an exploration to find an efficient anti-viral agent. From the previous scientific studies of traditional herbal medicines like garlic, ginger, onion, turmeric, chilli, cinchona and pepper, 131 chemical constituents were identified. The filtered search of drug-like-molecules searched using Datawarrior resulted in 13 active constituents (apoquinine, catechin, cinchonidine, cinchonine, cuprediene, epicatechin, epiprocurcumenol, epiquinine, procurcumenol, quinidine, quinine, zedoaronediol, procurcumadiol) showed no mutagenic, carcinogenic or toxic properties. *In silico* study of these 13 compounds with the best binding affinity towards SARS-CoV-2 protease was carried out. The ligands were subjected to molecular docking using Autodock Vina. Epicatechin and apoquine showed highest binding affinity of -7 and -7.5kcal/mol while catechin and epicatechin showed four hydrogen bond interactions. It is interesting and worth noticing the interaction of GLU166 residue with the ligand in most of the constituents. The effectiveness of catechin and epicatechin as an antiviral agent could be tested against COVID-19.

Keywords: COVID-19, Catechin, Epicatechin, Data Warrior, Molecular Docking, Plant Products