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Ensemble-based screening of natural products and FDA-approved drugs identified potent inhibitors of SARS-CoV-2 that work with two distinct mechanisms

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Abstract

The recent outbreak of SARS-CoV-2 is responsible for high morbidity and mortality rate across the globe. This requires an urgent identification of drugs and other interventions to overcome this pandemic. Computational drug repurposing represents an alternative approach to provide a more effective approach in search for COVID-19 drugs. Selected natural product known to have antiviral activities were screened, and based on their hits; a similarity search with FDA approved drugs was performed using computational methods. Obtained drugs from similarity search were assessed for their stability and inhibition against SARS-CoV-2 targets. Diosmin (DB08995) was found to be a promising drug that works with two distinct mechanisms, preventing viral replication and viral fusion into the host cell. Isoquercetin (DB12665) and rutin (DB01698) work by inhibiting viral replication and preventing cell entry, respectively. Our analysis based on molecular dynamics simulation and MM-PBSA binding free energy calculation suggests that diosmin, isoquercetin, rutin and other similar flavone glycosides could serve as SARS-CoV-2 inhibitor, hence an alternative solution to treat COVID-19 upon further clinical validation.

Keywords

SARS-CoV-2; COVID-19; Natural products; Docking screening; MD simulation; Free energy calculation