Comparative computational research on nanosized molecules of SARS-CoV-2 for validation of a verdant drug molecule

S. Hari Lakshmi and T. Devasena*

Centre for Nanoscience and Technology, Anna University, Chennai 600 025, India

The present study assesses cubebinol from *Piper cubeba* as a potential antiviral against SARS-CoV-2, comparing its efficacy to remdesivir. Docking studies show that cubebinol binds more effectively to the spike proteins and papain-like protease of SARS-CoV-2, with binding energies of –5.28, –7.46 and –7.39 kcal/mol respectively. Cubebinol demonstrates superior pharmacokinetics, including higher intestinal absorption and blood-brain barrier penetration, with no significant toxicological issues. The results suggest that cubebinol is a promising candidate for treating SARS-CoV-2 and should be further explored for clinical application.

Keywords: Cubebinol, docking, omicron, phytocomponents, SARS-CoV.

and acute respiratory syndrome and sometimes people even remained asymptomatic[2]. The standard drugs used to treat COVID-19 include hydroxychloroquine, an anti-malarial drug that prevents the replication of SARS-CoV-2 but has a few limitations. Other drugs used to treat COVID-19 have shown good responses in cell culture level and a combination of ribavirin and interferon is also recommended to treat SARS-CoV-2. A study has shown that an antiviral drug remdesivir previously used against Ebola virus can act against COVID-19 (ref. 3). Potential drug candidates for COVID-19 have already been reviewed[4]. As no proper medications or vaccines are being approved, molecular docking can serve as a reliable and potent tool to design a drug[5]. The screening of the drug and the target viral protein with known structures