Unraveling the antiviral activity of Stachytarpheta cayennensis against SARS-CoV-2 variants using in vitro and molecular docking analysis

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Abstract

The COVID-19 pandemic has emphasized the urgent need for new treatments for SARS-CoV-2, especially with the emergence of variants of concern. These variants can partially evade monoclonal therapeutic or neutralizing antibodies from natural infection or vaccination. Thus, identifying effective treatments against SARS-CoV-2 variants is crucial. Stachytarpheta cayennensis is known for its anti-inflammatory properties and has recently been used to treat COVID-19. In this study, we performed a chemical fractionation of the S. cayennensis extract and evaluated its viral entry inhibition activity using the pseudovirus method. UPLC-ESI-MS analysis was conducted to identify the active components in the fractions. Additionally, molecular docking simulations were performed to assess the effect of the compounds on the interaction between the SARS-CoV-2 spike protein and its human receptor, angiotensin-converting enzyme-2 (ACE2). Our findings revealed that the methanol extract and butanol fraction of S. cayennensis exhibited significant entry inhibitory activity against SARS-CoV-2 gamma and delta VOCs. 6-β-hydroxy-ipolamiide, ipolamiide, and verbascoside/isoverbascoside were identified as the prominent compounds in the butanol fraction. Molecular docking analysis revealed that 6-β-hydroxy-ipolamiide was the most potent inhibitor, while the other compounds also bound to the spike-ACE2 complex, contributing to an additive inhibitory effect. This study revealed the therapeutic potential of S. cayennensis in treating COVID-19 and provided valuable insights into the molecular mechanisms underlying its antiviral activity.