Title : In Silico Screening of binding inhibitors targeting spike protein of SARS-CoV-2

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ABSTRACT

The spread of SARS-CoV-2 has significantly impacted the treatment efficacy as the mutations manifested increasingly throughout the pandemic. New treatments have been urgently needed to combat the outbreak effectively. To this end, in silico screening methods and molecular docking have been employed to explore the potential of sesamin from sesame and marine natural product compounds in inhibiting the SARS-CoV-2 spike protein, a protein critical for viral entry. Several studies have indicated that sesame and natural product compounds contain numerous metabolites and potent antioxidants that are effective in antiviral activity and prevent allergic reactions. Therefore, this study aims to analyze the interactions and stability between sesamin derivatives and marine natural product compounds with the spike protein at the Tyr489 position. Molecular docking simulations and MM-PBSA binding energy calculations were employed to evaluate the compound potential as new SARS-CoV-2 inhibitors. A set of 6,142 compounds was obtained from the virtual chemical database, including 6,014 sesamin derivatives and 128 marine natural products. These compounds were then subjected to virtual screening, molecular dockings, and interaction analysis using molecular dynamics simulations. The studies revealed four ligand compounds, which are sesamin derivatives SE1 and SE2, and marine-derived natural products MA1 and MA2, showed the ability to bind to the spike protein, with ΔG values ranging from -31.14 to -16.43 kcal/mol. Notably, SE1, with ΔG values of -31.14 kcal/mol exhibits the highest potential for the further development as an effective antiviral drug against SARS-CoV-2.

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