

Title : Computational Study of Northern Thai Natural Product Compounds as Inhibitors for Main Protease of SARS-CoV-2 Omicron Variant

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ABSTRACT

The ongoing COVID-19 outbreak and the emergence of new variants, such as the Omicron variant, highlight the urgent need for identifying and developing effective inhibitory compounds or therapeutic drugs to combat the evolving virus and prevent further public health crises. A key target in developing antiviral treatments is the main protease of SARS-CoV-2, also known as Mpro or 3CLpro, which plays an essential role in viral replication. The enzyme is also absent in human cells, thus reducing the off-target effects arising from the antiviral inhibitors developed. This study evaluated the potential application of natural products from Northern Thailand in inhibiting Mpro, targeting the catalytic site at the His41 and Cys145 positions. A computational approach was employed, including molecular docking, drug-likeness analysis, MD simulations, and MMPBSA calculations. The results showed that Yokovanol has the lowest $\Delta G_{\text{binding}}$ of -28.81 ± 2.29 kcal/mol, better than the reference compound Baicalein, with $\Delta G_{\text{binding}}$ of -19.4 ± 2.38 kcal/mol. Energetic component analysis suggests that Yokovanol exhibits a strong potential to inhibit Mpro, highlighting its promise as a candidate for developing COVID-19 treatments. This study elucidates the potential and medicinal properties of plants from Northern Thailand, which have not been previously investigated in the context of antiviral drug development.

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