**Anti-Dengue Therapeutic Potential Of Vietnamese Herbal Formula: An Integrated *In Silico* And *In Vitro* Evaluation**

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**Background and aims.** Dengue Fever caused by the Dengue virus (DENV) has become a major public health concern, with no approved antiviral therapy currently available.1 Based on clinical manifestations, treatment protocols, and the traditional medicine theory, a Vietnamese herbal formula composed of six medicinal plants, including Bambusa vulgaris, Prunella vulgaris, Imperata cylindrica, Eclipta prostrata, Platycladus orientalis, and Lonicera japonica, has been considered as a potential treatment for Dengue fever.2 This formula has been previously applied in clinical settings, but it has not yet undergone rigorous scientific evaluation. Therefore, this study aimed to investigate this formula's antiviral activity against DENV through a combination of *in silico* and *in vitro* approaches to elucidate its mechanism of action.

**Methods.** Molecular docking was conducted by AutoDock Vina 1.1.2 for 201 phytochemicals derived from the herbal formula that met Lipinski’s Rule of Five into the NS5 methyltransferase (PDB: 4R8S). For the *in vitro* analysis, the neutralizing activity of the herbal extracts against all four DENV serotypes was evaluated using the Plaque Reduction Neutralization Test (PRNT50) using BHK-21 cells.

**Results.** Docking simulations showed that 41.3% of compounds exhibited strong binding affinities to NS5 MTase protein. These compounds were mainly belonged to the flavonoid, steroid, and terpenoid structural groups. PRNT50 assay results indicated that the aqueous extract had neutralizing activity with values ranging from 1002.5 to 8020 µg/mL, while the 40% ethanol extract showed stronger activity with PRNT50 values ranging from 256.2 to 512.5 µg/mL against all four DENV strains. The better antiviral activity potential of 40% ethanol extract was attributed to the presence of coumarins and a higher content of triterpenoids.

**Conclusion/Discussion.** In conclusion, traditional Vietnamese herbal formula for the treatment of dengue fever demonstrated the inhibitory activity against the DENV in both *in silico* and *in vitro* studies.

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**References:**

(1) Centers for Disease control and prevention. About Dengue: what you need to know (2024). URL: https://www.cdc.gov/dengue/about/index.html (accessed 2025-04-03).

(2) Bui, C. H.; Tran, K. Diseases and Treatment Based on Traditional Medicine Combined with Modern Medicine. Dong Nai Publishing, 1990.