2024.10.04-06

前沿轉譯與應用

第39屆 **第39屆** 第24屆 **天然藥物研討會** 台灣自由基學會學術研討會 聯合會暨國科會藥學及中醫藥學學門成果發表會 Cutting Edge, Translation and Application-Joint Symposium of the 39th SNP and 24th SFRR-Taiwan

摘要集 Abstract Book

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天然物化學組

Natural Products Chemistry



2024 Cutting Edge, Translation and Application-Joint Symposium of the 39th SNP and 24th SFRR-Taiwan

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PC-54

Phytochemical Investigation and Anti-COVID Screening of Compounds from *Bischofia javanica* Leaves

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The global impact of the coronavirus pandemic on human health, economy, and society has been profound. In this context, the search for potent anti-viral drugs has become an urgent necessity. *Bischofia javanica*, a plant species of the family Phyllanthaceae, has a rich traditional history of treating chronic conditions such as inflammation, tuberculosis, ulcers, fractures, and eczema. Furthermore, previous research studies have reported its potential secondary metabolite activities, such as anti-diabetic, anti-venom, sedative, and anti-cancer activities. This study, therefore, was aimed at isolating, determining the structure, and evaluating the bioactivities of *Bischofia javanica* leaves, including their potential as anti-COVID, anti-inflammatory, and cytotoxic agents, offering a ray of hope in the fight against the pandemic.

The strength of our research lies in our collaborative efforts. Pseudovirus assay (Omicron) was conducted for 75% aqueous methanol (75% MeOH) extract, and the results showed an IC50 value of $1.44 \pm 0.02 \mu g/mL$. Moreover, anti-inflammatory in human neutrophils were evaluated. The UPLC-HRMS/MS analysis of 75% MeOH extract revealed the presence of eight compounds, namely, gallic acid, hydroxybenzoic acid, methyl gallate, corilagin isomer,

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geraniin, ellagic acid, vitexin. Further, we conducted molecular docking studies to predict the binding mode and affinity of the compounds to the SARS-CoV-2 spike protein. This was followed by molecular dynamics simulations to study the behavior of the protein-ligand complex over time. Geraniin and corilagin bound well to the binding site with binding affinities of -7.0 and -6.1 kcal/mol and promising dynamics. In collaboration with researchers from Ukraine, we also analyzed plants of the genus *Epilobium* that are widely distributed in European countries and have a similar composition, including gallic acid, tannins, and flavonoids.

Keywords: tannins; phenolics; Jia-Dong; anti-COVID; molecular docking; dynamics