# *IN SILICO* DOCKING ANALYSIS OF *PHALERIA MACROCARPA* FRUIT PHYTOCHEMICALS IN INHIBITING SARS-COV-2

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## ABSTRACT

### *IN SILICO* DOCKING ANALYSIS OF *PHALERIA MACROCARPA* FRUIT PHYTOCHEMICALS IN INHIBITING SARS-COV-2

SARS-CoV-2, which has struck the world, has shocked society with its devastating death toll. Synthetic antivirals are commonly used but have the potential to cause serious side effects and long-term health problems. Consequently, there's a rising demand for natural antivirals due to their potential for fewer side effects and their promise of more sustainable treatments. *Phaleria macrocarpa* was reported to possess high antiviral properties due to the presence of the flavonoid compound such as quercetin, kaempferol, myricetin and naringenin. However, the antiviral properties of these compounds against SARS-CoV-2 have not yet been fully elucidated. Thus, the objectives of this study are to determine the phytochemicals of *P. macrocarpa* fruit using GC-MS analysis and phytochemical screening test, to evaluate the potential of the phytochemical in inhibiting SARS-CoV-2 via *in silico* docking analysis and also to determine the pharmacokinetics properties of its phytochemical using SWISSADME. In this study, the fruit of the *P. macrocarpa* was subjected to extraction using maceration method. Then, the phytochemical constituents in the fruit extract were identified using phytochemical screening and GC-MS analysis. The result obtained is positive for phytochemical screening test, however the GC-MS analysis showed less favorable results, whereby it just produced 7 peaks that have 90% of a quality. Among the 7, there's only one compound which is squalene that has antiviral properties. Thirteen phytochemical constituents were chosen from databases based on their potential in exhibiting the antiviral properties and were analyzed for their pharmacokinetic properties using SwissADME, which were aligned with the docking score obtained from PyRx. It was found that the potential compounds to inhibit SARS-CoV-2 were sesamin, Mahkoside A and Mahkoside B with docking score of -7.8, -7.4 and -7.5 respectively. This discovery of phytochemical constituents derived from P.macrocarpa fruit extract could potentially be developed as a natural alternative to existing medicines and vaccines currently available in the market.

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