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Computational study of SARS-CoV-2 M^{pro} inhibition by phytochemicals in five traditional medicinal plants

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Developing antiviral drugs against the current crisis of coronavirus disease 2019 (COVID-19), caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), is of high priority among scientific communities. The main viral protease enzyme (M^{pro}) is a key target of COVID-19 drugs, as the inhibition of which could halt disease progression. In search for potential inhibitors, phytochemicals from Sri Lankan traditional medicinal plants are an invaluable source of drug leads. Therefore, this study utilized molecular docking based virtual screening to evaluate the inhibition of SARS-CoV-2 M^{pro} by phytochemicals in five medicinal plants that formulate the traditional herbal preparation of 'paspanguwa'. A total of 15 phytochemicals were assessed for their pharmacokinetic properties *in-silico*, upon which, 9 favorable compounds were identified and were docked against the target using Autodock Vina engine in PyRx software. Evaluation of docking scores revealed three compounds, diosgenin, kaempferol and ecdysterone, as promising hits against M^{pro}. These three compounds exhibit low toxicity as well as high bioavailability. Upon binding to the enzyme, they formed favorable interactions with key residues in the active site. Hence, the results of this study indicated that diosgenin, kaempferol and ecdysterone could act as potential inhibitors of SARS-CoV-2 M^{pro}. These findings may provide new insights for developing antiviral therapeutics against SARS-CoV-2.

Keywords: SARS-CoV-2 M^{pro}, COVID-19, Traditional medicine, Phytochemicals

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