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LC-MS Based Metabolite Profiling of Ethanol Extract From the Sungkai (Peronema canescens Jack) and In Silico Prediction of Antidiabetic Activity With α-Glucosidase

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Abstract
Sungkai (Peronema canescens Jack) is a medicinal plant in the Verbenaceae family that is known to have antidiabetic activity. The secondary metabolite content found in sungkai leaves is in the form of alkaloids, flavonoids, triterpenoids, steroids, phenolics, and saponins. This research aimed to identify the biological activity of compounds in sungkai plants as antidiabetic agents using α-glucosidase inhibitors in silico. Sungkai leaf extract with ethanol solvent was identified using a Liquid Chromatography Mass Spectrometer (LC-MS/MS). There are 15 compounds resulting from LC-MS/MS analysis which will then predict antidiabetic activity using molecular docking. Molecular docking was carried out using AutoDock Tools software and visualized with Discovery Studio. The highest scoring result obtained from the molecular docking test was the compound C13H23N6S with a free bond energy result of-7.31 and an inhibition constant value of 4.41 μM, which binds three hydrogen bonds in GLU 78, ALA 75, and GLU 198.

Author Keywords
In sillico; metabolite profilling; Peronema canescens

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