Isolation of Antioxidant and Antibacterial Compounds from Extract of Teh-Tehan Leaf (*Acalypha Siamensis*) and Activity Approach Through *In Silico* Study

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Abstract

The increasing number of diseases caused by free radicals and bacterial infections that occur in developing countries as a cause of death problems in Indonesia. Indonesian native plant called Teh-tehan leaf has potential as a medicinal plant which has been used as an antibacterial at the extract stage. Isolation of active compounds needs to be done to identify the structure and activity so that the determination of the dose can be done.

Isolation of active compounds was carried out using thin layer chromatography methods with the silica gel stationary phase and the mobile phase of methanol: chloroform: hexane (7: 2: 1). The pure compounds that have been obtained are characterized by using UV / Vis and infrared spectrophotometers, as well as mass spectrometers and core magnetic resonance (NMR). Molecular docking is done using the PyRx program and visualized using the Discovery Studio program.

The results of the interpretation show the active compound (E) -3- (1H-indol-3-yl) -1- (4-methoxyphenyl) -prop-2-en-1-one. The compound has a very strong antioxidant activity with an IC_{50} value of 42.54369 ppm using the DPPH method. Antibacterial activity test showed moderate activity in S. aureus with inhibition zone values of 1.6-2 cm. *In silico* tests showed that the compound was able to interact well with protein superoxide dismutase (SOD), glutathione peroxidase (GPX), peptidoglycan glycosyltransferase (PGT) and D-alanyl-D-alanine carboxypeptidase (DACA) by inhibiting molecular docking (molecular docking).

Keywords: *Acalypha siamensis*, isolation, antioxidants, antibacterial, *molecular docking*