

ABSTRACT

Arumah Syarifatus Saniyah. 24020221130022. ***In Silico Study of Phytochemical Compounds of Milkwort (Polygala sp.) as Immunomodulatory Agents.*** Under the guidance of Hermin Pancasakti Kusumaningrum and Siti Roswiyah Yulyani.

Autoimmune disease is an abnormal immune response that attacks healthy tissue. In Indonesia, this disease affects more than 2.5 million people and caused more than 35,000 deaths in 2021. The administration of synthetic non-steroidal immunomodulatory drugs is toxic to the liver and kidneys. Phytochemical compounds in Polygala sp. possess anti-inflammatory activity and have the potential to inhibit the activity of TNF- α and interleukin-6 (IL-6), which play a role in autoimmune pathogenesis. This study aims to analyze and compare phytochemical compounds in several Polygala species that have potential as immunomodulatory agents and inhibitors of TNF- α and IL-6 activity through in silico molecular docking studies. The methods employed included collecting GC-MS data from Polygala vulgaris, P. rosmarinifolia, and P. javana through a literature review, preparing test receptors and ligands, determining the active sites of receptor proteins, docking the test ligands, visualizing the docking results, conducting Lipinski's pharmacology test, and analyzing the data. Molecular docking results showed that the binding affinity of the control ligand to TNF- α was -9.4 kcal/mol, while that to IL-6 was -6.5 kcal/mol. In P. vulgaris, the compound N-isobutyl-dodecatetraenamide exhibits the strongest binding affinity for TNF- α and IL-6, at -6.2 kcal/mol and -5.5 kcal/mol, respectively. In P. rosmarinifolia, the compound with the strongest binding affinity is benzene, 1,2-dimethoxy-4-[[4-methylphenyl)sulfonyl]methyl]-, with a binding affinity of -7.4 kcal/mol for TNF- α and -6.4 kcal/mol for IL-6. Meanwhile, P. javana contains the compound spiro[androst-5-ene-17,1'-cyclobutan]-2'-one, 3-hydroxy-, (3 β ,17 β) with a binding affinity of -9.5 kcal/mol against TNF- α ; the compounds 1H-perimidine, 2,3-dihydro-2-(2,4,5-trimethoxyphenyl)- and 4H-1-benzopyran-4-one, 5-hydroxy-2-(4-hydroxyphenyl)-3,7-dimethoxy-, with binding affinities of -7.1 and -7.0 kcal/mol for IL-6, respectively. The compounds from these three species meet the Lipinski 5-rule pharmacology test.

Keywords: Polygala sp., TNF- α , IL-6, autoimmune, molecular docking