

ABSTRAK

MUHAMAD GHAZI YUSGHIFARI ZALDI, 2024. NETWORK PHARMACOLOGY DAUN PULAI (*Alstonia scholaris* L.) SEBAGAI ANTIASMA, SKRIPSI, PROGRAM STUDI S1 FARMASI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA. Dibimbing oleh Dr. apt. Rina Herowati, M.Si. dan apt. Jena Hayu Widyasti, M.Farm.

Asma adalah penyakit heterogen klinis pada saluran napas bawah yang ditandai dengan peradangan kronis dan hiperaktivitas saluran napas yang menyebabkan batuk, mengi, kesulitan bernapas, dan dada terasa sesak. Daun pulai berpotensi sebagai antiasma. Tujuan penelitian ini untuk mengetahui protein-protein target yang terlibat dalam patofisiologi asma, mengetahui senyawa dalam daun pulai yang diprediksi menjadi target kerja dari protein target dalam patofisiologi asma, dan untuk mengetahui profil *network pharmacology* kandungan senyawa kimia daun pulai terhadap protein target asma.

Penelitian ini menggunakan metode *network pharmacology* pengumpulan data kandungan senyawa-senyawa kimia daun pulai daun pulai menggunakan KNApSACk, dan jurnal-jurnal penelitian. Protein target yang terlibat dalam patofisiologi penyakit asma diidentifikasi menggunakan KEGG *pathway* dan jurnal penelitian. Protein target dilakukan validasi nama protein menggunakan UniProt. Interaksi protein-protein menggunakan String. Skrining zat aktif terhadap protein target dengan Pubchem. Prediksi protein target dari senyawa bioaktif menggunakan Swiss Target Prediction, SEA, dan SuperPred. Visualisasi *network pharmacology* dari interaksi protein-protein dan interaksi senyawa-protein menggunakan Cytoscape.

Visualisasi profil *network pharmacology* protein target yang terlibat dalam patofisiologi asma dengan senyawa daun pulai yaitu NFKB1, GSK3B, SYK, BLNK, BTK, GRB2, LAT, LCK, MAP2K1, RAF1, PIK3CA, dan FYN. Kandungan senyawa *akuammicine*, *betulinic acid*, *oleanolic acid*, *ursolic acid*, *beta-sitosterol*, *isorhamnetin*, *stigmasterol*, *chlorogenic acid*, *quercetin*, *citral*, *tetrahydroalstonine*, *alpha-amyrin*, dan *kaempferol* pada daun pulai dapat membentuk profil *network pharmacology* dengan protein target asma.

Kata kunci : asma, daun pulai, *network pharmacology*, Cytoscape

ABSTRACT

MUHAMAD GHAZI YUSGHIFARI ZALDI, 2024. NETWORK PHARMACOLOGY OF PULAI LEAVES (*Alstonia scholaris* L.) AS ANTI-ASTHMA, THESIS, S1 PHARMACY STUDY PROGRAM, FACULTY OF PHARMACY, SETIA BUDI UNIVERSITY, SURAKARTA. Supervised by Dr. apt. Rina Herowati, M.Sc. and apt. Jena Hayu Widyasti, M.Farm.

Asthma is a clinical heterogeneous disease of the lower respiratory tract characterized by chronic inflammation and hyperactivity of the airways that causes coughing, wheezing, difficulty breathing, and chest tightness. Pulai leaves have the potential as antiasthmatics. The purpose of this study was to determine the target proteins involved in the pathophysiology of asthma, to determine the compounds in pulai leaves that are predicted to be the target of the target proteins in the pathophysiology of asthma, and to determine the network pharmacology profile of the chemical compounds in pulai leaves against asthma target proteins.

This study uses the network pharmacology method of collecting data on the chemical compounds of pulai leaves using KNApSack, and research journals. Target proteins involved in the pathophysiology of asthma were identified using the KEGG pathway and research journals. Target proteins were validated by protein name using UniProt. Protein-protein interactions using String. Screening of active substances against target proteins with Pubchem. Prediction of target proteins from bioactive compounds using Swiss Target Prediction, SEA, and SuperPred. Visualization of network pharmacology of protein-protein interactions and compound-protein interactions using Cytoscape.

Visualization of network pharmacology profiles of target proteins involved in the pathophysiology of asthma with pulai leaf compounds, namely NFKB1, GSK3B, SYK, BLNK, BTK, GRB2, LAT, LCK, MAP2K1, RAF1, PIK3CA, and FYN. The content of akuammicine, betulinic acid, oleanolic acid, ursolic acid, beta-sitosterol, isorhamnetin, stigmasterol, chlorogenic acid, quercetin, citral, tetrahydroalstonine, alpha-amyrin, and kaempferol compounds in pulai leaves can form a network pharmacology profile with asthma target proteins.

Keyword : asthma, pulai leaves, network pharmacology, Cytoscape