# ABSTRAK


PREDIKSI KANDIDAT SENYAWA HASIL ISOLASI DARI KULIT BATANG *Sesbania grandiflora* (L.) SEBAGAI ANTI-INFLAMMASI COVID-19 MENGGUNAKAN ANALISIS *NETWORK PHARMACOLOGY, MOLECULAR DOCKING,* DAN *MOLECULAR DYNAMICS SIMULATIONS*

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Turi putih (*S. grandiflora*) merupakan salah satu tumbuhan asli Indonesia yang biasa dimanfaatkan sebagai anti-inflammasi. Tujuan penelitian ini adalah untuk mendapatkan senyawa yang potensial sebagai anti-inflammasi COVID-19 menggunakan analisis *Network Pharmacology, Molecular Docking,* dan *Molecular Dynamics Simulations.* Senyawa yang berhasil diisolasi dari kulit batang turi putih dan target proteinnya diperoleh melalui proses *data mining,* dan dibuat jaringan senyawa-target protein. Selanjutnya, jaringan target protein untuk penyakit inflammasi COVID-19 juga dibuat agar dapat digabungkan dengan jaringan senyawa-target protein. Selanjutnya, jaringan *Protein-Protein Interaction* (PPI) dibangun, berdasarkan target protein yang mengalami *overlapping*. Target protein dengan nilai *degree* tertinggi secara berurutan adalah SRC, MAPK1, HSP90AA1, PIK3R1, AKT1, RELA, JAK2, PTPN11, NFKB1, ERBB2 dengan nilai *degree* masing-masing yakni 23, 19, 17, 17, 16, 14, 14, 13, 13, dan 11. Setelah itu, dilakukan *filtering* berdasarkan topologi *degree, betwenness centrality,* dan *closeness centrality,* untuk mendapat target protein paling signifikan dengan hasil target protein SRC, MAPK1, PIK3R1, HSP90AA1, dan AKT1. Berdasarkan GO & KEGG *Enrichment Analysis,* target protein signifikan kebanyakan berasosiasi dengan anotasi *Biological Processes response to hormone* dan KEGG *Pathway* yakni MAPK *signalling pathway* & PIK3-Akt *signalling pathway* dalam *pathway in cancer*. Berdasarkan validasi *Molecular Docking,* senyawa sesbagrandiflorain A memiliki energi ikatan terbaik sebesar -9 kcal/mol dengan membentuk 3 ikatan hidrogen pada LYS 295 (4,65 Å), THR 338 (5,41 Å), PHE 405 (3,10 Å) dengan target protein SRC serta stabil selama *Molecular Dynamics Simulations* berdasarkan nilai rata-rata RMSD & RMSF masing-masing sebesar 1,1 Å dan 0,65 Å.



Kata kunci: *S. grandiflora*, anti-inflammasi, COVID-19, *Network Pharmacology, Molecular Docking, Molecular Dynamics Simulations*

## ABSTRACT

PREDICTION OF CANDIDATE COMPOUNDS ISOLATED FROM *Sesbania grandiflora* (L.) STEM BARK AS ANTI-INFLAMMATORY COVID-19 USING NETWORK PHARMACOLOGY ANALYSIS, MOLECULAR DOCKING, AND MOLECULAR DYNAMICS SIMULATIONS

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White turi (*S. grandiflora*) is a native Indonesian plant which is commonly used as an anti-inflammatory. The aim of this study was to obtain potential compounds as anti-inflammatory for COVID-19 using Network Pharmacology, Molecular Docking, and Molecular Dynamics Simulations analysis. Compounds that were successfully isolated from the stem bark of white turi and their protein targets were obtained through a data mining process, and a compound-protein target network was made. Furthermore, the protein target network for the inflammatory disease COVID-19 was also made so that it could be combined with the protein target compound network. A Protein-protein interaction (PPI) network is constructed based on the overlapping protein targets. The protein targets with the highest degree values sequentially are SRC, MAPK1, HSP90AA1, PIK3R1, AKT1, RELA, JAK2, PTPN11, NFKB1, ERBB2 with respective degree values of 23, 19, 17, 17, 16, 14, 14, 13, 13, and 11. After that, filtering was carried out based on topology degree, betweenness centrality, and closeness centrality, to get the most significant protein targets with the results of protein targets SRC, MAPK1, PIK3R1, HSP90AA1, and AKT1. Based on GO & KEGG Enrichment Analysis, significant protein targets are mostly associated with the annotation of Biological Processes response to hormone and KEGG Pathway namely MAPK signalling pathway & PIK3-Akt signalling pathway in pathway in cancer. Based on Molecular Docking validation, sesbagrandiflorin A has the best bond energy of -9 kcal/mol by forming 3 hydrogen bonds at LYS 295 (4.65 Å), THR 338 (5.41 Å), PHE 405 (3.10 Å) with SRC protein targets and stable during Molecular Dynamics Simulations based on RMSD & RMSF mean values of 1.1 Å and 0.65 Å, respectively.



Keywords: *S. grandiflora*, anti-inflammatory, COVID-19, Network Pharmacology, Molecular Docking, Molecular Dynamics Simulations