

ABSTRAK

ISOLASI DAN IDENTIFIKASI SENYAWA METABOLIT SEKUNDER DARI FRAKSI POLAR DAUN SUNGKAI (*Peronema Canescens* Jack) SERTA STUDI POTENSI ANTIVIRUS *SEVERE ACUTE RESPIRATORY SYNDROME CORONAVIRUS 2* (SARS-COV-2) SECARA *IN SILICO*

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Tumbuhan sungkai (*Peronema canescens* Jack) merupakan tumbuhan tingkat tinggi yang umumnya digunakan masyarakat Indonesia sebagai obat tradisional. Daun tumbuhan ini memiliki khasiat sebagai antikanker, antibakteri, antimalaria, dan antiinflamasi. Penelitian ini bertujuan untuk mengisolasi dan mengidentifikasi senyawa metabolit sekunder dari fraksi polar daun sungkai, serta pengujian isolat sebagai antivirus SARS-CoV-2 secara *in silico*. Tahapan penelitian yang dilakukan meliputi ekstraksi, proses pemurnian menggunakan metode kromatografi kolom, karakterisasi, dan *molecular docking* secara *in silico*. Senyawa yang berhasil diisolasi berupa kristal kuning pucat (NV26) sebanyak 3,7 mg. Identifikasi struktur senyawa hasil isolasi dilakukan dengan metode ¹H-NMR dan ¹³C-NMR. Berdasarkan analisis data spektroskopi, senyawa NV26 diperkirakan sebagai senyawa flavonoid dengan rumus molekul C₁₆H₁₂O₅. Kajian potensi sebagai antivirus dari senyawa NV26 dilakukan dengan metode *docking* menggunakan program *Autodock 4.2* dan *Autodock vina*. Berdasarkan *docking* yang dilakukan, NV26 berhasil membentuk ikatan dengan makromolekul SARS-Cov-2 *Macro Domain* (7CZ4) dan *Cryo-EM Struktur SARS-CoV-2 Omicron BA.1 Spike Protein* (8DMA) serta memiliki potensi sebagai inhibitor enzim SARS-Cov-2 Mpro.

Kata kunci : Daun Sungkai, *peronema canescens*, flavonoid, *in silico*, SARS-CoV-2 Mpro, *molecular docking*

ABSTRACT

ISOLATION AND IDENTIFICATION OF SECONDARY METABOLITE COMPOUNDS FROM POLAR FRACTION OF SUNGKAI LEAVES (*Peronema canescens* JACK) AND IN SILICO STUDY OF THE POTENTIAL FOR ANTIVIRUS SEVERE ACUTE RESPIRATORY SYNDROME CORONAVIRUS 2 (SARS-COV-2)

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Sungkai plant (*Peronema canescens* Jack) is higher plant that is generally used by Indonesian people as traditional medicine. The leaves of this plant have properties such as being anti-cancer, antibacterial, anti-malaria, and anti-inflammantory. This study aims to isolate and identify secondary metabolite compounds from the polar fraction of Sungkai leaves, as well as isolate them for testing as an in silico SARS-CoV-2 antivirus. Stage of research carried out include extraction, purification process using coloum chromatography, characterization, and in silico molecular docking. The compound that was successully isolated was in the form of pale yellow crystals (NV26) containing 3,7 mg, identification of isolated compound stucture was carried out using the ¹H-NMR and ¹³C-NMR methods. Based on spectroscopic data analysis, the compound NV26 is estimated to be a flavonoid compound with the molecular formula C₁₆H₁₂O₅. The study of the potential as an antivirus of the NV26 compound was carried out by the docking method using the Autodock 4.2 and Autodock vina programs. Based on docking carried out, NV26 managed to form bonds with the macromolecular of SARS-CoV-2 Macro Domain (7CZ4) and the cryo-EM structure of SARS-CoV-2 omicron BA 1 spike protein (8DMA) and has potential as an enzyme inhibitor for SARS-CoV-2 Mpro.

Key words : Sungkai leaves, *peronema canescens*, flavonoid, in silico, SARS-CoV-2 Mpro, molecular docking