ABSTRAK

ISOLASI DAN IDENTIFIKASI SENYAWA METABOLIT SEKUNDER DARI FRAKSI DAUN SUNGKAI (*Peronema canescens* Jack) SERTA STUDI POTENSI ANTIINFLAMASI SECARA *IN VITRO* DAN *IN SILICO*

Oleh

Ofriani Fatrika

Tumbuhan Sungkai (*Peronema canescens* Jack) terutama bagian daun sungkai sering dimanfaatkan oleh masyarakat Indonesia sebagai obat tradisional, rebusan daun sungkai sering digunakan untuk meningkatkan imunitas tubuh, menurunkan demam, menurunkan kadar asam urat, sebagai obat antimalaria, antivirus dan antibakteri.

Penelitian ini bertujuan untuk mengisolasi dan mengidentifikasi senyawa metabolit sekunder dari fraksi daun sungkai serta kajian potensi antiinflamasi secara *in vitro* dan *in silico.* Tahapan penelitian meliputi maserasi, partisi, uji antiinflamasi secara *in vitro,* isolasi menggunakan metode kromatografi cair vakum, kromatografi kolom, dan kromatografi lapis tipis. Karakterisasi senyawa menggunakan *Liquid Chromatography-Mass Spectrometry* (LCMS/MS). Kajian secara *in silico* dilakukan dengan metode *molekuler docking* menggunakan *AutoDock Vina*.

Berdasarkan uji antiinflamasi secara *in vitro,* fraksi etil asetat memiliki aktivitas antiinflamasi yang lebih baik dari fraksi *n*-heksana dan fraksi diklorometana, nilai IC_{50} yang diperoleh sebesar 52,12 µg/mL. Berdasarkan hasil analisis LCMS/MS didapatkan rumus molekul $C_{16}H_{12}O_5$ diduga sebagai senyawa flavonoid yaitu acacetin dan diberi kode NV37. Uji antiinflamasi secara *in silico,* hasil *docking* senyawa NV37 terhadap reseptor 3LN1 dan 5KIR berhasil membentuk ikatan dengan diperolehnya nilai afinitas ikatan sebesar -8,78 kkal/mol dan -6,16 kkal/mol. Nilai afinitas ikatan yang negatif menandakan bahwa senyawa NV37 memiliki potensi sebagai inhibitor enzim COX-2.

Kata kunci : Daun sungkai, flavonoid, *in silico,* inflamasi, *molecular docking*.

ABSTRACT

ISOLATION AND IDENTIFICATION OF SECONDARY METABOLITE COMPOUNDS FROM SUNGKAI LEAVES FRACTIONS (*Peronema canescens* Jack) AND STUDY OF IN VITRO AND IN SILICO ANTIINFLAMMATORY POTENTIAL

By

Ofriani Fatrika

The Sungkai plant (*Peronema canescens* Jack), especially the sungkai leaves, is often used by Indonesian people as traditional medicine. Decoction of sungkai leaves is often used to increase body immunity, reduce fever, reduce uric acid levels, as an antimalarial, antiviral and antibacterial drug.

This research aims to isolate and identify secondary metabolite compounds from sungkai leaves fractions as well as study antiinflammatory potential in vitro and in silico. The research stages included maceration, partitioning, in vitro antiinflammatory testing, isolation using vacuum liquid chromatography, column chromatography and thin layer chromatography. Compound characterization using Liquid Chromatography-Mass Spectrometry (LCMS/MS). In silico studies were carried out using the molecular docking method using AutoDock Vina.

Based on in vitro antiinflammatory tests, the ethyl acetate fraction had better antiinflammatory activity than the *n*-hexane fraction and the dichloromethane fraction, the IC_{50} value obtained was 52.12 µg/mL. Based on the results of LCMS/MS analysis, it was found that the molecular formula $C_{16}H_{12}O_5$ was thought to be a flavonoid compound, namely acacetin and was given the code NV37. In silico antiinflammatory tests, the docking results of the NV37 compound against the 3LN1 and 5KIR receptors succeeded in forming bonds with binding affinity values of -8.78 kcal/mol and -6.16 kcal/mol. Negative binding affinity value indicates that the NV37 compound has potential as a COX-2 enzyme inhibitor.

Key words: Sungkai leaves, flavonoids, in silico, inflammation, molecular docking.