

## ABSTRAK

### IDENTIFIKASI DAN ISOLASI SENYAWA BIOAKTIF ANTIINFLAMASI DARI KULIT BATANG TUMBUHAN TURI PUTIH (*Sesbania grandiflora* (L.) Poir) MENGGUNAKAN METABOLOMIK BERBASIS LC-MS/MS

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Turi putih (*S. grandiflora*) merupakan salah satu tumbuhan asli Indonesia yang biasa dimanfaatkan sebagai antiinflamasi. Tujuan penelitian ini mendapatkan senyawa bioaktif antiinflamasi dari hasil isolasi menggunakan metabolomik berbasis LC-MS/MS. Senyawa hasil isolasi didapatkan melalui ekstraksi dengan variasi konsentrasi pelarut MeOH 100%, EtOAc 100% dan MeOH:EtOAc 50% dengan uji antiinflamasi menggunakan metode penghambatan denaturasi protein. Aktivitas antiinflamasi yang paling baik diperoleh dari ekstrak EtOAc 100% dengan rata-rata nilai IC<sub>50</sub> sebesar 117,54 µg/mL. Dari hasil analisis LC-MS/MS didapatkan 106 senyawa *known* dan 394 senyawa *unknown*. Ekstrak sampel kulit batang tumbuhan turi putih dikelompokkan berdasarkan variasi pelarut pengekstrak melalui analisis *partial component analysis* (PCA) dengan total *primary component* (PC) 83% saat menggunakan data luas area dan 60% saat menggunakan data intensitas. Data LC-MS/MS yang berupa luas area dan intensitas dikorelasikan dengan aktivitas antiinflamasi menggunakan *orthogonal partial least squares-discriminant analysis*. Hasil analisis OPLS-DA menunjukkan bahwa senyawa 36 (Sesbgrandiflorain C), senyawa 44 (Sesbgrandiflorain B) dan senyawa 84 (2-metil-5-{2-[2-(4-metil-3,6-dioksosikloheksa-1,4-dienil)etoksi]etil}benzo-1,4 quinon) merupakan metabolit penciri *known* yang diduga berkontribusi *major* (utama) pada aktivitas antiinflamasi ekstrak kulit batang tumbuhan turi putih. Senyawa murni berhasil diisolasi dari ekstrak etil asetat 100% kulit batang tumbuhan turi putih melalui kromatografi cair vakum (KCV) dan kromatografi kolom gravitasi (KKG). Isolat yang beraktivitas antiinflamasi diperoleh berupa kristal kuning sebanyak 7,2 mg dan 5 mg diduga sebagai senyawa sesbgrandiflorain C dan sesbgrandiflorain B berdasarkan hasil analisis dari LC-MS/MS serta OPLS-DA.

Kata Kunci: *S. grandiflora*, metabolomik, antiinflamasi, LC-MS/MS, PCA, OPLS-DA

## ABSTRACT

### IDENTIFICATION AND ISOLATION BIOACTIVE ANTI-INFLAMMATORY COMPOUNDS FROM THE STEAM BARK OF TURI WHITE PLANT (*Sesbania grandiflora* (L.) Poir) USING METABOLOMIC-BASED ON LC-MS/MS

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White turi (*S. grandiflora*) is one native Indonesian plant which is commonly used as an anti-inflammatory. The aim of this study was to obtain anti-inflammatory bioactive compounds from the results of isolation based on LC-MS/MS-based metabolomics. The isolated compounds were obtained by extraction with varying concentrations of 100% MeOH, 100% EtOAc and 50% MeOH:EtOAc with anti-inflammatory tests using the protein denaturation inhibition method. The best anti-inflammatory activity was obtained from 100% EtOAc extract with an average  $IC_{50}$  value of 117.54  $\mu\text{g/mL}$ . From the results of the LC-MS/MS analysis, 106 known compounds and 394 unknown compounds were obtained. The results of the LC-MS/MS analysis, 106 known compounds and 394 unknown compounds were obtained. Extract samples of turi putih stem bark were grouped based on variations in extracting solvents through partial component analysis (PCA) with a total primary component (PC) of 83% when using area data and 60% when using intensity data. LC-MS/MS data in the form of area and intensity were correlated with anti-inflammatory activity using orthogonal partial least squares-discriminant analysis. The results of the OPLS-DA analysis showed that compound 36 (sesbagrandidflorain C), compound 44 (sesbagrandidflorain B) and compound 84 (2-methyl-5-{2-[2-(4-methyl-3,6-dioxocyclohexa-1,4)dienyl]ethoxy}ethyl}benzo-1,4-quinone) is a known characteristic metabolite which is thought to contribute majorly to the anti-inflammatory activity of turi putih stem bark extract. The pure compound was isolated from 100% ethyl acetate extract of the bark of the turi putih plant by means of vacuum liquid chromatography (KCV) and gravity column chromatography (KKG). Isolates with anti-inflammatory activity were obtained in the form of yellow crystals of 7.2 mg and 5 mg suspected as sesbagrandidflorain C and sesbagrandidflorain B based on the analysis results from LC-MS/MS and OPLS-DA.

Keywords: *S. grandiflora*, metabolomic, anti-inflammatory, LC-MS/MS, PCA, OPLS-DA