IDENTIFIKASI DAN KARAKTERISASI SENYAWA AKTIF DARI DAUN PELAWAN (*Tristaniopsis merguensis* Griff.) SEBAGAI ANTIBAKTERI

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INTISARI

Tujuan penelitian ini adalah untuk mengidentifikasi senyawa antibakteri dari ekstrak daun pelawan *Tristaniopsis merguensis*. Isolasi senyawa dilakukan melalui proses maserasi bertingkat berdasarkan kepolaran pelarut *n*-heksana, etil asetat, dan metanol. Hasil dari proses ekstraksi kemudian diuji aktivitas antibakteri menggunakan metode difusi cakram terhadap *Staphylococcus aureus* dan *Escherichia coli*. Ekstrak dengan potensi aktivitas antibakteri tertinggi dipisahkan menggunakan kromatografi kolom dan kemudian fraksi hasil pemisahan diuji kembali terhadap aktivitas antibakteri. Identifikasi senyawa aktif dari fraksi dengan aktivitas antibakteri tertinggi dilakukan menggunakan *Liquid Chromatography–High Resolution Mass Spectrometer* (LC-HRMS). Studi penambatan molekul terhadap protein 3G7B (*S. aureus*) dan 1KZN (*E. coli*) digunakan untuk memperkirakan mekanisme aksi senyawa dalam fraksi dengan aktivitas antibakteri tertinggi.

Hasil uji antibakteri menunjukkan bahwa ekstrak etil asetat memiliki aktivitas lebih baik dibandingkan dengan ekstrak metanol dan *n*-heksana, dengan nilai *Minimum Inhibition Concentration* (MIC) masing-masing terhadap bakteri *S. aureus* dan *E. coli* adalah sebesar 2500 µg/mL dan 10000 µg/mL. Analisis LC-HRMS mengindikasikan bahwa ekstrak etil asetat mengandung senyawa flavonoid sebagai senyawa utama. Fraksi hasil kromatografi kolom dengan kode PE4.9.8 memiliki aktivitas antibakteri dengan nilai zona hambat terhadap *S. aureus* sebesar 6 mm. Hasil analisis LC-MS/MS terhadap fraksi PE4.9.8 menunjukkan kandungan senyawa *sugiresinol*, *4,4'-(5-hydroxytetrahydro-2H-pyran-2,4-diyl)diphenol*, dan *butin* (6). Hasil analisis *in silico* terbaik ditunjukkan oleh senyawa *5,7-dihidroxy-2-(3-hidroxyphenyl)-6,8-dimethylchroman-4-one* (9) terhadap protein 3G7B *(S. aureus)* dengan nilai energi ikatan sebesar -8,1 kkal/mol, dan senyawa *7-methoxy-5-3'-4'-trihydroxyflavone* (4) terhadap protein 1KZN *(E. coli)* dengan nilai energi ikatan sebesar -7,6 kkal/mol.

Kata kunci: Ekstraksi, daun, *Tristaniopsis merguensis*, LC-HRMS, antibakteri.

IDENTIFICATION AND CHARACTERIZATION OF ACTIVE COMPOUNDS FROM THE LEAVES OF PELAWAN (*Tristaniopsis merguensis* Griff.) AS ANTIBACTERIAL

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ABSTRACT

The aim of this research was to identify antibacterial compounds from Tristaniopsis merguensis pelawan leaf extract. Compound isolation was carried out through a multistage maceration process based on the polarity of the solvents n-hexane, ethyl acetate, and methanol. The results of the extraction process were then tested for antibacterial activity using the disc diffusion method against *Staphylococcus aureus* and *Escherichia coli.* The extract with the highest potential antibacterial activity was separated using column chromatography, and then the separated fraction was tested again for antibacterial activity. Identification of active compounds from the fraction with the highest antibacterial activity was carried out using a Liquid Chromatography-High-Resolution Mass Spectrometer (LC-HRMS). Molecular docking studies of the 3G7B (*S. aureus*) and 1KZN (*E. coli*) proteins were used to estimate the mechanism of action of compounds in the fraction with the highest antibacterial activity.

Antibacterial test results show that ethyl acetate extract has better activity compared to methanol and *n*-hexane extracts, with Minimum Inhibition Concentration (MIC) values against *S. aureus* and *E. coli* bacteria of 2.500 µg/mL and 10.000 µg/mL, respectively. LC-HRMS analysis indicated that the ethyl acetate extract contained flavonoids as the main compound. The column chromatography fraction with code PE4.9.8 has antibacterial activity with an inhibition zone value against S. aureus of 6 mm. The results of LC-MS/MS analysis of the PE4.9.8 fraction showed that it contained the compounds sugiresinol, 4,4'-(5-hydroxytetrahydro-2H-pyran-2,4-diyl)diphenol, and butin (6). The best in silico analysis results were shown by the compound 5,7-dihydroxy-2-(3-hydroxyphenyl)-6,8-dimethylchroman-4-one (9) against the 3G7B (*S. aureus*) protein with a bond energy value of -8.1 kcal/mol, and the compound 7-methoxy-5-3'-4'-trihydroxyflavone (4) against the 1KZN protein (*E. coli*) with a bond energy value of -7.6 kcal/mol.

Keywords: Extraction, leaf, *Tristaniopsis. merguensis*, LC-HRMS, and antibacterial.