

**STUDI *IN SILICO* PEPTIDA ANTIMIKROBA
DARI KAYU SECANG (*Caesalpinia sappan* L.)
TERHADAP *Klebsiella pneumoniae***

SKRIPSI

**HANIF FARID SUDJUD
A221016**



**SEKOLAH TINGGI FARMASI INDONESIA
YAYASAN HAZANAH
BANDUNG
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Sebagai salah satu syarat untuk memperoleh gelar Sarjana Farmasi

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Juli 2026

Disetujui oleh:

Pembimbing

A handwritten signature in black ink, appearing to be 'Umi Baroroh', with a stylized, cursive script.

Umi Baroroh, S.Si., M.Biotek.

Pembimbing

A handwritten signature in blue ink, appearing to be 'Himalaya Wana Kelana', with a stylized, cursive script. To the right of the signature, the date '29/7' is written.

Himalaya Wana Kelana, M.Pd.

Kutipan atau saduran baik sebagian atau seluruh naskah, harus menyebut nama pengarang dan sumber aslinya, yaitu Sekolah Tinggi Farmasi Indonesia.

Skripsi ini saya persembahkan untuk kedua orang tua dan keluarga saya yang selalu memberikan doa yang tak pernah putus, kerja keras tanpa mengeluh, serta pengorbanan yang sering tak terlihat namun selalu saya rasakan. Setiap langkah yang saya capai hari ini adalah buah dari doa dan usaha kalian yang tak pernah berhenti.

ABSTRAK

Klebsiella pneumoniae merupakan bakteri Gram-negatif anggota ESKAPE yang resistensinya terhadap antibiotik terus meningkat. Kondisi ini menuntut alternatif terapi baru seperti peptida antimikroba. Penelitian ini bertujuan mengidentifikasi dan mengevaluasi kandidat peptida antimikroba dari kayu secang terhadap tiga protein target *K. pneumoniae* yaitu OmpA, SHV-1 β -laktamase, dan OmpK36. Penelitian dilakukan melalui pendekatan *in silico*. Tahapan penelitian meliputi identifikasi peptida dari sekuens protein kayu secang serta prediksi aktivitas antimikroba, sifat fisikokimia, sifat biologis, dan profil ADMET. Struktur tiga dimensi peptida diprediksi dan divalidasi sebelum ditambatkan pada protein target dengan meropenem dan VvK1 sebagai kontrol. Dari tujuh peptida yang diuji, peptida LGITK dan LGITKT terpilih sebagai dua kandidat terbaik. Keduanya memiliki aktivitas antimikroba spesifik, sifat fisikokimia stabil, profil biologis dan ADMET yang aman, serta struktur tiga dimensi tervalidasi baik. Kedua peptida menunjukkan interaksi molekuler dan afinitas ikatan yang baik terhadap seluruh protein target. Peptida LGITKT secara konsisten lebih unggul dan SHV-1 β -laktamase merupakan target paling prospektif karena afinitas ikatan kedua peptida melampaui kontrol meropenem dan VvK1. Temuan ini menunjukkan bahwa peptida LGITK dan LGITKT merupakan kandidat peptida antimikroba potensial terhadap *K. pneumoniae*.

Kata kunci: antimikroba, *Caesalpinia sappan* L., *Klebsiella pneumoniae*, peptida

ABSTRACT

Klebsiella pneumoniae is a Gram-negative bacterium of the ESKAPE group whose resistance to antibiotics continues to increase, demanding new therapeutic alternatives such as antimicrobial peptides. This study aimed to identify and evaluate candidate antimicrobial peptides derived from sappan wood (*Caesalpinia sappan* L.) against three *K. pneumoniae* target proteins, namely OmpA, SHV-1 β -lactamase, and OmpK36. The research was conducted using an *in silico* approach. The stages included identification of peptides from sappan wood protein sequences, followed by prediction of antimicrobial activity, physicochemical properties, biological properties, and ADMET profile. Three-dimensional peptide structures were predicted and validated prior to docking onto the target proteins, with meropenem and VvK1 used as controls. Of the seven peptides tested, LGITK and LGITKT were selected as the two best candidates. Both exhibited specific antimicrobial activity, stable physicochemical properties, safe biological and ADMET profiles, and well-validated three-dimensional structures. Both peptides demonstrated favorable molecular interactions and binding affinities toward all target proteins. LGITKT consistently outperformed LGITK, and SHV-1 β -lactamase was identified as the most prospective target, as the binding affinities of both peptides exceeded those of the meropenem and VvK1 controls. These findings indicated that LGITK and LGITKT were potential antimicrobial peptide candidates against *K. pneumoniae*.

Keywords: antimicrobial, *Caesalpinia sappan* L., *Klebsiella pneumoniae*, peptide

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