ABSTRAK

ANGGITA DWI RISTANTI, 2024. ANALISIS PENAMBATAN MOLEKULER DAN PREDIKSI PROFIL ADMET SENYAWA KULIT TANAMAN KAYU MANIS *(Cinnamomum cassia)* SEBAGAI KANDIDAT OBAT KANKER PARU-PARU, SKRIPSI, PROGRAM STUDI S1 FARMASI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA. Dibimbing oleh Dr. apt. Rina Herowati, M.Si. dan apt. Dwi Ningsih, M.Farm.

Kanker paru-paru merupakan salah satu kanker paling umum dan penyebab utama kematian secara global. Terapi konvensional seperti kemoterapi dan pembedahan memiliki risiko efek samping yang tinggi, sehingga diperlukan alternatif seperti pengobatan herbal. Kayu manis (*Cinnamomum cassia*) diketahui mengandung senyawa aktif yang berpotensi sebagai antikanker. Penelitian ini bertujuan memprediksi interaksi senyawa kulit kayu manis terhadap target protein kanker paru-paru serta mengevaluasi profil farmakokinetik dan toksisitasnya.

Metode meliputi penyaringan senyawa berdasarkan drug-likeness, validasi metode docking menggunakan *PyMOL* (RMSD), dan docking otomatis dengan *SwissDock*. Visualisasi interaksi ligan-protein dilakukan menggunakan *LigPlot+*. Senyawa hasil docking terbaik kemudian dianalisis profil farmakokinetik dan toksisitasnya secara *in silico*.

Hasil menunjukkan beberapa senyawa memiliki afinitas ikatan yang baik dan berinteraksi pada binding pocket yang sesuai dengan ligan asli. Senyawa *5'-methoxylariciresinol*, rosavin, kumarin, *(+)-isolariciresinol*, dan evofolin B menunjukkan interaksi yang kuat. Prediksi ADMET menunjukkan *evofolin* B, *(+)-isolariciresinol*, dan rosavin memiliki absorpsi, distribusi, metabolisme, ekskresi yang baik serta toksisitas rendah. Ketiga senyawa ini berpotensi sebagai kandidat antikanker paru-paru.

Kata kunci : Kanker paru-paru, Kayu manis, Penambatan molekuler, Senyawa antikanker.

ABSTRACT

ANGGITA DWI RISTANTI, 2024. MOLECULAR DOCKING ANALYSIS AND ADMET PROFILE PREDICTION OF COMPOUNDS FROM CINNAMON BARK (*Cinnamomum cassia*) AS POTENTIAL LUNG CANCER DRUG CANDIDATES, THESIS, BACHELOR OF PHARMACY STUDY PROGRAM, FACULTY OF PHARMACY, SETIA BUDI UNIVERSITY, SURAKARTA. Supervised by Dr. apt. Rina Herowati, M.Si. and apt. Dwi Ningsih, M.Farm.

Lung cancer is one of the most common types of cancer and a leading cause of death worldwide. Conventional therapies such as chemotherapy and surgery often carry high risks of side effects, prompting the need for alternative treatments such as herbal medicine. Cinnamon (Cinnamomum cassia) is known to contain active compounds with potential anticancer properties. This study aims to predict the interaction of cinnamon bark compounds with lung cancer target proteins and to evaluate their pharmacokinetic and toxicity profiles.

The method involved compound screening based on drug-likeness, docking method validation using PyMOL (RMSD), and automated docking with SwissDock. Ligand-protein interaction visualization was conducted using *LigPlot+*. The top docking compounds were then analyzed for their pharmacokinetic and toxicity profiles *in silico*.

The results showed that several compounds exhibited strong binding affinities and interacted within the binding pocket similar to the native ligand. The compounds *5'-methoxylariciresinol*, rosavin, kumarin, *(+)-isolariciresinol*, and evofolin B demonstrated favorable interaction. ADMET predictions indicated that evofolin B, *(+)-isolariciresinol*, and rosavin possess good absorption, distribution, metabolism, and excretion properties with low toxicity. These three compounds are predicted to be potential candidates for lung cancer therapy.

Keywords: Lung cancer, Cinnamon, Molecular docking, Anticancer compounds