SKRIPSI

STRUCTURE-BASED VIRTUAL SCREENING (SBVS) SENYAWA TANAMAN OBAT DALAM AL-QUR'AN DAN AL-HADITS DENGAN TERGET RESEPTOR HISTAMIN H_2 SEBAGAI ANTI-*GASTROINTESTINAL DISEASE*

DISUSUN OLEH :

AFRILIYANA ISMY ASTY

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PROGRAM STUDI S1 FARMASI

SEKOLAH TINGGI ILMU KESEHATAN 'AISYIYAH

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Skripsi ini Diajukan sebagai
Salah Satu Syarat untuk Memperoleh Gelar
Sarjana Farmasi (S.Farm)

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Structure-Based Virtual Screening* (SBVS) Senyawa Tanaman Obat Dalam Al-Qur'an Dan Al-Hadits Dengan Target Reseptor Histamin H_2 Sebagai Anti-*Gastrointestinal Disease

ABSTRAK

Latar belakang: Reseptor histamin yang penting pada manusia salah satunya yaitu reseptor histamin H_2, berperan dalam regulasi reseptor asam lambung. Menurut WHO tahun 2014, di Indonesia angka kematian akibat penyakit tukak lambung mencapai 1.081 atau 0,08% dari total kematian. Penelitian ini melakukan skrining struktur-struktur tanaman bahan alam yang disebutkan dalam al-Quran dan al-Hadits dengan target reseptor histamin H_2 diharapkan mampu mengidentifikasi ligan-ligan yang berperan sebagai antihistamin H_2, khususnya untuk penyakit *gastrointestinal.* **Tujuan:** Melakukan penapisan secara virtual senyawa-senyawa dalam tanaman obat yang disebutkan dalam al-Qur'an dan al-Hadits dengan target reseptor histamin H_2, Melakukan simulasi dinamika molekul pada kompleks hasil penapisan virtual dan menghitung energi bebas ikatan paling stabil, dan melakukan validasi internal kompleks paling stabil dengan simulasi penambatan ulang. **Metode:** Penelitian ini melakukan uji *in silico* dengan metode simulasi penambatan molekul, simulasi dinamika molekul, dan penambatan ulang menggunakan perangkat lunak YASARA-*Structure* dan Autodock vina **Hasil:** SBVS pada ligan tanaman dalam al-Qur'an dan al-Hadits terhadap reseptor histamin H_2 manusia, didapatkan tanaman Safarjal dengan kode LTS0117717 memiliki interaksi yang baik terhadap reseptor H_2, ditandai dengan nilai energi bebas ikatan paling rendah -8,1 kkal/mol, terbentuknya ikatan hidrogen dengan Asp98 berat molekul tidak >500DA yaitu 456,7DA. Hasil simulasi dinamika molekul dengan 20ns terpilih *snapshoot* ke 154 karena nilai energi bebas ikatan paling rendah yaitu -11.3810 kj/mol dan mempunyai jarak antar ikatan <3,5Å yaitu 1,850Å. Hasil penambatan ulang memiliki nilai RMSD 100% <2Å yaitu berkisar 0.6923Å-1.0290Å. **Kesimpulan:** Tanaman Safarjal dengan kode LTS0117717 yaitu senyawa Oleanolic acid, disinyalir memiliki efek farmakologis terhadap reseptor histamin H_2 manusia sebagai anti-*gastointestinal disease*.

Kata Kunci : Al-Quran dan Al-Hadits, *Gastrointestinal*, SBVS, $hHRH_2$, Komputasi.

HIGH SCHOOL OF HEALTH SCIENCES 'AISYIYAH PALEMBANG S1 PHARMACEUTICAL STUDY PROGRAM

Skripsi, July 2023

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Structure-Based Virtual Screening (SBVS) Of Medicinal Plant Compounds In The Al-Qur'an And Al-Hadith By Targeting Histamine H_2 Receptors As Anti-*Gastrointestinal Disease*

ABSTRACT

Background: One of the important histamine receptors in humans, the histamine H2 receptor, plays a role in the regulation of stomach acid receptors. According to WHO in 2014, in Indonesia the death rate due to peptic ulcer disease reached 1,081 or 0.08% of the total deaths. This study screened the plant structures of natural materials mentioned in the al-Qur'an and al-Hadith with the target of histamine H_2 receptors expected to be able to identify ligands that act as H_2 antihistamines, especially for gastrointestinal diseases. **Objectives:** Virtually screening compounds in medicinal plants mentioned in the al-Qur'an and al-Hadith targeting histamine H_2 receptors, simulating molecular dynamics in virtual filtration complexes and calculating the most stable bond-free binding energy, and performing internal validation of the most stable complexes by simulating re-docking. **Methods:** This research conducted in silico tests with molecular docking simulation methods, molecular dynamics simulation, and re-docking. **Results:** SBVS on plant ligands in the Qur'an and al-Hadith against human histamine H_2 receptors, it was found that the Safarjal plant with code LTS0117717 had good interactions with H_2 receptors, characterized by the lowest binding free energy value of -8.1 kcal/ mole, hydrogen bonds are formed with Asp98, the molecular weight is not >500DA, namely 456.7DA. The results of the molecular dynamics simulation with 20ns selected the 154th snapshoot because the bond free energy value is the lowest, namely -11.3810 kj/mol and has an inter-bond distance of <3.5Å, namely 1.850Å. The re-docking results have a 100% RMSD value <2Å, namely around 0.6923Å-1.0290Å. **Conclusion:** The Safarjal plant with the code LTS0117717, namely the compound Oleanolic acid, is suspected to have a pharmacological effect on human histamine H_2 receptors as an anti-gastointestinal disease.

Keywords : Al-Qur'an and Al-Hadith, Gastrointestinal, SBVS, $hHRH_2$, computational

DAFTAR ISI

BAB V

KESIMPULAN DAN SARAN

A. Kesimpulan

Telah diteliti sebanyak 33 tanaman yang disebutkan dalam al-Qur'an dan al-Hadits, terpilih satu tanaman terbaik yang disinyalir sebagai anti-*gastrointestinal*, yaitu tanaman Safarjal dengan kode LTS0117717, berikut alasan terpilihnya kode LTS0117717 nama senyawanya yaitu Oleanolic acid.

1. Pada SBVS menggunakan Autodock vina menghasilkan dengan energi bebas ikatan paling rendah -8,1 Kkal/mol, berat molekul kurang dari 500DA yaitu 456,7 DA, dan berikatan dengan Asp98.
2. Pada simulasi dinamika molekul menggunakan 20ns terpilih *snapshoot* ke 154, karena mempunyai *pose* yang paling stabil yang ditandai dengan nilai energi bebas ikatan paling rendah yaitu -11.3810 kj/mol, dan mempunyai jarak antar ikatan <3,5Å yaitu 1,850Å.
3. Hasil *re-docking* 1000x didapatkan nilai RMSD <2Å dengan persentase 100% yaitu berkisar 0.6923Å-1.0290Å.

B. Saran

Disarankan bahwa bisa dilakukan penelitian lebih lanjut lagi mengenai tanaman Safarjal sebagai anti-*gastointestinal disease*.

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