SKRIPSI

PENCARIAN KANDIDAT SENYAWA OBAT DARI TANAMAN BAHAN ALAM DI INDONESIA DENGAN TARGET RESEPTOR ADRB-2 (PDB:2RH1) SEBAGAI ANTIASMA DENGAN METODE *STRUCTURE-BASED VIRTUAL SCREENING* (SBVS)

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Skripsi, Juni 2023

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Pencarian Kandidat Senyawa Obat Dari Tanaman Bahan Alam Di Indonesia Dengan Target Reseptor ADRB-2 (PDB:2rh1) Sebagai Antiasma Dengan Metode *Structure-Based Virtual Screening* (SBVS)

ABSTRAK

Latar Belakang: Penyakit asma merupakan penyakit yang banyak diderita manusia, di Indonesia sendiri pada tahun 2018 sebanyak 2,4% masyarakat Indonesia menderita penyakit asma data tersebut dari kemenkes RI. Reseptor yang berperan dalam penyakit asma yaitu ADRB-2. Penemuan dan pengembangan obat baru dengan menggunakan tanaman bahan alam merupakan hal penting untuk menghasilkan produk-produk yang bermanfaat di dunia Kesehatan. Pencarian obat baru dengan sedikit atau tanpa efek samping merupakan alasan penting, sehingga terjadi peningkatan minat penggunaan produk alami untuk mengobati antiinflamasi dan nyeri.
Tujuan: Melakukan penapisan secara virtual senyawa-senyawa dalam tanaman obat di Indonesia dengan target reseptor ADRB-2 (PDB:2RH1), 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 menlakukan uji *in silico* dengan metode simulasi penambatan molekul, simulasi dinamika molekul, dan penambatan ulang.
Kesimpulan: Tanaman kecubung dengan pengkodean LTS0110348 berpotensi sebagai antiasma karena memiliki energi bebas ikatan paling rendah, berat molekul <500DA, jarak antar ikatan <3,5Å, berikatan dengan asam amino Asn312, dan memiliki nilai RMSD <2Å.

Kata kunci: SBVS, simulasi dinamika molekul, penambatan ulang, ADRB-2, asma, tanaman bahan alam.

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ABSTRACT

Background: Asthma is a disease that many humans suffer from, in Indonesia alone in 2018 as many as 2.4% of Indonesians suffered from asthma the data from Ministry of Health of the Republic of Indonesia. The receptor that plays a role in asthma is ADRB-2. The discovery and development of new drugs using natural plants is important to produce useful products in the world of health. The search for new drugs with few or no side effects is an important reason, resulting in an increased interest in the use of natural products to treat anti-inflammatories and pain.
Objective: Virtually screening compounds in medicinal plants in Indonesia with ADRB-2 receptor target (PDB:2RH1), simulating molecular dynamics in the virtual filtration complex and calculating the most stable bond-free energy, and performing internal validation of the most stable complex by simulating re-docking.
Method: This study conducted *in silico* tests with molecular tethering simulation methods, molecular dynamics simulation, and re-docking.
Conclusion: Datura metel plant with LTS0110348 coding has potential as an antiasthma because it has the lowest bond-free energy, molecular weight <500DA, bond distance <3.5Å, binding to amino acid Asn312, and has an RMSD value of <2Å.

Keywords: SBVS, molecular dynamics simulation, re-docking, ADRB-2, asthma, plant natural material.

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BAB V

KESIUMPULAN DAN SARAN

A. Kesimpulan

Dari 40 tanaman yang diteliti yang berpotensi sebagai antiasma, terpilih satu tanaman yang terbaik yaitu, tanaman kecubung dengan pengkodean LTS0110348 dengan energi bebas ikatan paling rendah -12,7 Kkal/mol, berat molekul kurang dari 500DA, berikatan dengan asam amino Asn312. Beberapa asam amino yang berikatan dengan reseptor ADRB-2 antara lain, Asp113, Thr118, Ser203, Asn293, Asn312, dan Tyr316, pada penelitian ini ikatan vital yang terbentuk adalah Asn312.

Pada simulasi dinamika molekul menggunakan 30ns terpilih pdb interval ke 190 karena mempunyai *pose* yang paling stabil ditandai dengan nilai energi bebas ikatan paling rendah yaitu -13,9600 kj/mol, mempunyai jarak antar ikatan < 3,5Å yaitu 2,5 Å. Hasil *re-docking* 1000x didapatkan nilai RMSD <2Å yaitu dengan rentang nilai 0,8-1,02Å.

B. Saran

Disarankan bahwa bisa dilakukan penelitian lebih lanjut lagi mengenai tanaman kecubung sebagai antiasma.

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