ABSTRAK

Penambatan Molekul Senyawa Flavonoid Jantung Pisang *(Musa sp.)* sebagai Inhibitor DPP-4 yang Berpotensi Memberikan Efek Antidiabetes

Oleh :
Nanda Fajri Zamroni
11181165

Diabetes melitus 2 diakibatkan adanya kelainan metabolisme tubuh akibat defisiensi tubuh dalam memproduksi insulin atau resistensi insulin. DPP-4 merupakan protein yang sangat berpengaruh dalam regulasi insulin. Penggunaan obat antidiabetes seperti DPP-4 inhibitor, dengan mekanisme mencegah perombakan *incretin* GLP-1 dan GIP oleh protein DPP-4. Maka dari itu subyek protein ini sangat populer dikalangan peneliti untuk dicari senyawa-senyawa yang berpotensi memberikan efek antidiabetes. Penelitian ini bertujuan menentukan apakah dari 12 senyawa flavonoid pilihan dapat menginhibisi protein target berdasarkan hasil parameter docking dan jenis ikatan yang diberi. Penelitian dilakukan menggunakan metode *docking*. Senyawa uji dan protein uji dipreparasi, dioptimasi dan diuji penambatan molekulnya. Didapatkan senyawa terbaik S4 (Hesperetin Dihydrochalcone) dengan binding affinity -6,3 kcal/mol, ki 24,09 mikromolar yang berikatan hidrogen dengan target residu TYR A:547. Binding affnity S4 masih rendah dibandingkan dengan ligand alami (Vildagliptin). Maka dari itu senyawa belum berpotensi sebagai antidiabetes.

Kata Kunci : docking molekuler, flavonoid, DPP-4, antidiabetes, vildagliptin, konstanta inhibisi, energi bebas.

ABSTRACT

Molecular Docking of Flavonoid compounds from Banana Flower (Musa acuminata) as DPP-4 Inhibitor

By:
Nanda Fajri Zamroni
11181165

Diabetes mellitus 2 is caused by metabolic disorders due to the body's deficiency in producing insulin or insulin resistance. DPP-4 is a protein that is very influential in insulin regulation. The use of antidiabetic drugs such as DPP-4 inhibitors, with the mechanism of preventing the breakdown of GLP-1 and GIP incretins by DPP-4 proteins. Therefore, this protein subject is very popular among researchers to look for compounds that have the potential to provide antidiabetic effects. This study aims to determine whether the 12 selected flavonoid compounds can inhibit the target protein based on the results of docking parameters and the type of bond given. The research was conducted using the docking method. Test compounds and test proteins were prepared, optimized and tested for molecular docking. The best compound S4 (Hesperetin Dihydrochalcone) was obtained with a binding affinity of -6.3 kcal/mol, ki 24.09 micromolar which forms a hydrogen bond with the target TYR residue A:547. The binding affinity of S4 is still low compared to the natural ligand (Vildagliptin). Therefore, the compound has no potential as an antidiabetic.

Keywords: molecular docking, flavonoid, DPP-4, antidiabetic, vildagliptin, inhibitory effect, Gibbs free energy.