POTENSI KARAGENAN DARI ALGA MERAH (*RHODOPHYTA)* SEBAGAI KANDIDAT ANTIDIABETES TIPE 2 MENGGUNAKAN SIMULASI *MOLECULAR DOCKING*

SKRIPSI

Diajukan untuk memenuhi Sebagian dari syarat memperoleh gelar Sarjana Sains
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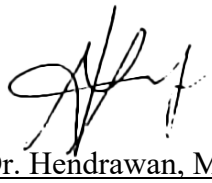

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ABSTRAK

Pada penelitian ini dilakukan kajian potensi karagenan dari alga merah (*Rhodophyta)* sebagai kandidat antidiabetes tipe 2 menggunakan simulasi *molecular docking.* Tahapan penelitian meliputi preparasi protein, preparasi ligan, validasi metode *docking*, proses *docking*, dan visualisasi hasil dengan menggunakan AutoDock Tools 1.5.6, AutoDock Vina 1.1.2, PyMOL 2.2.3, dan BIOVIA *Discovery Studio Visualizer* 2021. Melalui simulasi ditentukan afinitas pengikatan, interaksi molekuler, serta sifat inhibisi κ-karagenan dan ι-karagenan terhadap empat enzim yang berperan dalam regulasi karbohidrat, yaitu α-amilase, α-glukosidase, dipeptidil peptidase-IV (DPP-IV), dan glukosa-6-fosfat dehidrogenase (G6PD). Pembanding yang digunakan adalah akarbosa (inhibitor enzim α-amilase dan enzim α-glukosidase), linagliptin (inhibitor enzim DPP-IV) dan polidatin (inhibitor enzim G6PD). Hasil penelitian menunjukan bahwa κ-karagenan dan ι-karagenan dapat membentuk ikatan dengan semua enzim. Interaksi yang terjadi pada κ-karagenan dan ι-karagenan terhadap keempat enzim meliputi ikatan hidrogen, interaksi van der waals, interaksi hidrofobik, interaksi elektrostatik dan interaksi *unfavorable*. Afinitas pengikatan ι-karagenan lebih tinggi dari κ-karagenan terhadap α-amilase, sedangkan untuk α-glukosidase, DPP-IV, dan G6PD afinitas pengikatan κ-karagenan lebih tinggi dari ι-karagenan. Berdasarkan hasil penelitian diketahui bahwa κ-karagenan menginhibisi α-amilase, α-glukosidase, DPP-IV, dan G6PD, tapi tidak sebaik kontrol positif inhibitornya dengan selisih afinitas terhadap kontrol positifnya berturut-turut 0,1; 1,0; 1,7; dan 1 (*kkal/mol*). ι-karagenan menginhibisi α-amilase dengan baik, menginhibisi α-glukosidase, DPP-IV, dan G6PD, tapi tidak sebaik kontrol positif inhibitornya dengan selisih afinitas terhadap kontrol positifnya berturut-turut 0; 1,5; 5,5; dan 1,1 (*kkal/mol*). Dengan demikian κ-karagenan dan ι-karagenan berpotensi sebagai kandidat antidiabetes tipe 2. Pengujian lanjutan secara *in vivo* dan *in vitro* diperlukan untuk mendukung data simulasi yang diperoleh.

Kata Kunci: antidiabetes, inhibitor, karagenan, mikroalga, *molecular docking.*

ABSTRACT

This research aims to study the potential of carrageenan from red algae (*Rhodophyta*) as a candidate for type 2 antidiabetic using molecular docking. The research stages include protein preparation, ligand preparation, docking method validation, docking process, and visualization of results using AutoDock Tools 1.5.6, AutoDock Vina 1.1.2, PyMOL 2.2.3, and BIOVIA *Discovery Studio Visualizer* 2021. The binding affinity, molecular interactions, and the inhibitory properties of κ-carrageenan and ι-carrageenan were determined against four enzymes involved in carbohydrate regulation, namely α-amylase, α-glucosidase, dipeptidyl peptidase-IV (DPP-IV), and glucose-6-phosphate dehydrogenase (G6PD). The potency of carrageenan was evaluated by comparing with acarbose (inhibitor of α-amylase and α-glucosidase enzymes), linagliptin (inhibitor of DPP-IV enzyme) and polydatin (inhibitor of G6PD enzyme). The results showed that κ-carrageenan and ι -carrageenan could form bonds with all enzymes. The interactions that occur in κ-carrageenan and ι-carrageenan to the four enzymes include hydrogen bonding, van der waals interactions, hydrophobic interactions, electrostatic interactions and unfavorable interactions. The binding affinity of ι-carrageenan was higher than that of κ-carrageenan for α-amylase, while for α-glucosidase, DPP-IV, and G6PD the binding affinity of κ-carrageenan was higher than that of ι-carrageenan. Based on the results of the study, it was found that κ-carrageenan inhibited α-amylase, α-glucosidase, DPP-IV, and G6PD, but not as well as the positive control inhibitor with the difference in affinity for the positive control, respectively 0.1; 1.0; 1.7; and 1 (kcal/mol). ι-carrageenan inhibited α-amylase well, inhibited α-glucosidase, DPP-IV, and G6PD, but not as well as the positive control inhibitor with affinity differences for the positive control respectively 0; 1.5; 5.5; and 1.1 (kcal/mol). Therefore, κ-carrageenan and ι-carrageenan are potential candidates for type 2 antidiabetic. Further in vivo and in vitro testing is needed to support the obtained simulation data.

Keywords: antidiabetic, carrageenan, inhibitor, microalgae, molecular docking.

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