KAJIAN POTENSI PEPTIDA AKTIF DARI KOLAGEN KULIT IKAN NILA (*OREOCHROMIS NILOTICUS*) SEBAGAI KANDIDAT ANTIDIABETES TIPE-2 BERDASARKAN STUDI *MOLECULAR DOCKING*

SKRIPSI

diajukan untuk memenuhi sebagian syarat memperoleh gelar Sarjana Sains
Program Studi Kimia

oleh

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Sebuah skripsi yang diajukan untuk memenuhi salah satu syarat memperoleh gelar Sarjana Sains pada Fakultas Pendidikan Matematika dan Ilmu Pengetahuan Alam

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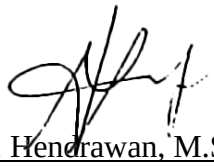

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ABSTRAK

Pada penelitian ini dilakukan kajian potensi peptida aktif dari kolagen kulit ikan nila (*Oreochromis niloticus*) sebagai kandidat antidiabetes tipe-2 berdasarkan studi *molecular docking.* Tahapan penelitian meliputi hidrolisis kolagen secara enzimatik menggunakan BIOPEP; seleksi peptida aktif; analisis toksisitas, alergenitas, dan sensori peptida aktif; serta simulasi pengikatan peptida aktif dengan enzim target DM tipe-2. Pembanding yang digunakan yaitu akarbosa, linagliptin, dan polidatin. Hasil hidrolisis kolagen secara *in silico* menghasilkan tiga belas (13) peptida aktif yang tidak bersifat toksik, non-alergen, serta berasa pahit, asin, dan sebagian tidak terdeteksi. Interaksi molekuler antara enzim α-amilase, α-glukosidase, DPP-IV, dan G6PD dengan peptida aktif melibatkan ikatan hidrogen, gaya van der Waals, interaksi hidrofobik, elektrostatik, pi-sulfur, dan *unfavorable*. Afinitas pengikatan peptida WF, WY, dan VW dengan α-amilase lebih tinggi 1,7; 1,6; dan 0,8 *kkal/mol* dibandingkan akarbosa. Kompleks α-glukosidase dengan WF, WY, VW, AF, SF, TF, VF, WG, PPG, RM, PG, PM, dan MG lebih tinggi daripada akarbosa dengan selisih berturut-turut 2,7; 2,6; 2,2; 2,1; 2; 1,9; 1,8; 1,8; 1,7; 1,2; 1; 0,8; dan 0,2 *kkal/mol*. Kompleks DPP-IV dengan WF, VW, WY, dan WG lebih tinggi 0,8; 0,5; 0,4; dan 0,3 *kkal/mol* daripada linagliptin. Kompleks G6PD dengan WF, WY, TF, VW, SF, PPG, VF, AF, dan WG lebih tinggi dibandingkan polidatin dengan selisih 1,2; 1,1; 0,7; 0,7; 0,6; 0,5; 0,5; 0,4; dan 0,4 *kkal/mol*. Peptida aktif menghambat keempat enzim secara kompetitif. Berdasarkan hasil penelitian dapat disimpulkan bahwa peptida aktif dari kolagen kulit ikan nila berpotensi sebagai kandidat antidiabetes tipe-2. Pengujian lebih lanjut secara *in vitro* dan *in vivo* perlu dilakukan untuk mendukung prediksi potensi yang diperoleh melalui pemodelan *molecular docking*.

Kata kunci: antidiabetes, ikan nila, inhibitor, *molecular docking*, peptida aktif

ABSTRACT

This study aims to evaluate the potential of active peptides from tilapia skin collagen (*Oreochromis niloticus*) as a candidate for type-2 antidiabetic based on molecular docking. Research stages include enzymatic hydrolysis of collagen using BIOPEP; active peptides selection; toxicity, allergenicity, and sensory analysis of active peptides; and binding simulation of active peptides with type-2 DM target enzymes. The potency of target compounds were compared with acarbose, linagliptin, and polydatin. In silico collagen hydrolysis generates thirteen (13) active peptides that were non-toxic, non-allergenic, bitter-taste, salty, and undetectable-taste. All active peptides interact with α-amylase, α-glucosidase, DPP-IV, and G6PD through hydrogen bonds, van der Waals, hydrophobic, electrostatic, pi-sulfur, and unfavorable interactions. The binding affinity of WF, WY, and VW peptides with α-amylase were 1.7; 1.6; and 0.8 *kcal/mole* higher than those of acarbose. The α-glucosidase complex with WF, WY, VW, AF, SF, TF, VF, WG, PPG, RM, PG, PM, and MG was higher than that of acarbose with energy difference of 2.7; 2.6; 2.2; 2.1; 2; 1.9; 1.8; 1.8; 1.7; 1,2; 1; 0.8; and 0.2 *kcal/mole*, respectively. The DPP-IV complex binding affinity with WF, VW, WY, and WG was higher 0.8; 0.5; 0.4; and 0.3 *kcal/mole* than linagliptin. The G6PD complex with WF, WY, TF, VW, SF, PPG, VF, AF, and WG was higher than polydatin with energy difference of 1.2; 1.1; 0.7; 0.7; 0.6; 0.5; 0.5; 0.4; and 0.4 *kcal/mole*. All active peptides inhibit the four enzymes competitively. All in all, it can be concluded that the active peptides from tilapia skin collagen have the potential to be used as antidiabetic type-2 candidates. Further in vivo and in vitro evaluation needs to be carried out to support the molecular docking findings.

Keywords: active peptides, antidiabetic, inhibitor, nile tilapia, molecular docking

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