IDENTIFIKASI PEPTIDA INHIBITOR α-AMILASE DARI HIDROLISAT KASEIN SUSU KAMBING SECARA *IN SILICO* DAN UJI AKTIVITASNYA

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INTISARI

Susu kambing memiliki potensi dalam pengobatan beberapa penyakit, salah satunya adalah mencegah terjadinya diabetes melitus tipe 2. Aktivitas ini dapat berasal dari protein susu kambing yang mengalami hidrolisis selama proses pencernaan menghasilkan peptida. Penelitian ini bertujuan untuk mengidentifikasi urutan asam amino peptida bioaktif inhibitor α-amilase dari hidrolisat kasein susu kambing secara *in silico* untuk disintesis dan menguji aktivitas inhibisi peptida terhadap α-amilase.

Peptida diperoleh dari urutan asam amino kasein susu kambing yang dihidrolisis secara *in silico digestion*. Peladen komputasi seperti Expasy Peptide Mass digunakan untuk *in silico digestion*. Peladen pendukung seperti Peptide Ranker dan PepSite 2 digunakan untuk prediksi peptida bioaktif. Peptida tersebut ditambatkan terhadap α-amilase. Peladen HADDOCK, CABS-dock, dan PepSite 2 digunakan untuk prediksi interaksi protein-peptida. Peptida hasil penambatan diuji aktivitas inhibisinya terhadap α-amilase untuk memperoleh nilai IC_{50}.

Berdasarkan studi *in silico digestion* diperoleh beberapa peptida yang diprediksi memiliki sifat bioaktif. Penambatan molekuler dilakukan untuk menentukan interaksi peptida terhadap α-amilase. Berdasarkan penambatan molekuler diprediksi 2 peptida bioaktif yang berpotensi untuk menginhibisi α-amilase, yaitu “EDVPSER” dan “TNAIPYVR”. Hasil uji aktivitas menunjukkan bahwa kedua peptida menunjukkan aktivitas dalam menginhibisi α-amilase. Peptida “EDVPSER” dapat menginhibisi kinerja α-amilase dengan nilai IC_{50} sebesar 14,16 ± 0,65 µM. Sementara itu, peptida “TNAIPYVR” juga menunjukkan inhibisi terhadap kinerja α-amilase dengan nilai IC_{50} sebesar 76,58 ± 2,13 µM.

Kata kunci: α-amilase, *in silico digestion*, penambatan molekuler, peptida.

IDENTIFICATION OF α-AMYLASE INHIBITOR PEPTIDE FROM GOAT'S MILK CASEIN HYDROLYZATE BY IN SILICO AND ITS ACTIVITY ASSAY

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ABSTRACT

Goat's milk has the potential to treat several diseases, for instance is preventing type 2 diabetes mellitus. This activity come from goat's milk protein which undergoes hydrolysis during the digestive process to produce peptides. This research aimed to identify the amino acid sequence of bioactive of α-amylase inhibitor peptide from goat's milk casein hydrolyzate by in silico to be synthesized and tested inhibitory activity of the peptide against α-amylase.

Peptides were attained from amino acid sequence of goat's milk casein that hydrolyzed by in silico digestion. Computational server including Expasy Peptide Mass was utilized for in silico digestion. Supporting server including Peptide Ranker and PepSite 2 were utilized to predict the bioactive peptide. Those peptides were docked to α-amylase. HADDOCK server, CABS-dock, and PepSite 2 server were utilized to predict protein-peptide interactions. Inhibitory activity of the docking result of bioactive peptide was analysed to obtain the IC_{50} value.

Based on in silico digestion study, several peptides were predicted to have bioactive activity. Molecular docking was conducted to determine the interaction of peptide against α-amylase. Based on molecular docking, 2 bioactive peptides were potentially inhibiting α-amylase, namely "EDVPSER" and "TNAIPYVR". The result of activity assay was revealed that both peptides performed an inhibitory activity against α-amylase. "EDVPSER" peptide could inhibit the performance of α-amylase with the IC_{50} value of 14,16 ± 0,65 μM. Meanwhile, "TNAIPYVR" peptide was also revealed the inhibition of α-amylase performance with the IC_{50} value of 76,58 ± 2,13 μM.

Keywords: α-amylase, in silico digestion, molecular docking, peptide.