Mengidentifikasi Peptida Bioaktif Angiotensin Converting Enzyme-inhibitor (ACEi) dari Kasein ÃŽÂ² Susu Kambing dengan Polimorfismenya Melalui Teknik In Silico

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Abstract	Susu kambing memiliki komponen protein salah satunya protein ÃŽÂ² dan secara umum terjadi polimorfisme pada level protein. Perubahan urutan asam amino akibat polimorfisme memungkinkan adanya potensi dihasilkannya peptida bioaktif penghambat enzim pengubah angiotensin (ACEi). Penelitian ini bertujuan untuk menyaring peptida bioaktif yang berpotensi sebagai ACEi dari kasein ÃŽÂ² kambing beserta polimorfismenya. Penelitian ini dilakukan dengan teknik in silico terhadap sekuen kasein ÃŽÂ² kambing serta struktur tiga dimensi human testicular ACE. Langkah yang dilakukan dalam penelitian ini meliputi simulasi pemotongan peptida dengan enzim pencernaan (pepsin, tripsin dan kimotripsin), peninjauan karakteristik peptida lalu simulasi docking ligan-reseptor. Tampilan parameter LipinskiÃ¢Â€Â™s Rule of Five (Ro5), bioaktivitas dan energi afinitas dipertimbangkan untuk memilih peptida bioaktif. Hasil yang didapat menunjukkan bahwa ditemukan peptida bioaktif yakni INK (Ile-Asp-Lys) yang memiliki kemampuan hampir setara dengan lisinopril (afinitas energi -8,2kkal/mol vs. -8,3kkal/mol). Peptida INK dapat ditemukan dari hasil hidrolisis dari alel A, C, D dan E, sehingga polimorfisme tidak menyebabkan perbedaan produksi peptida bioaktif. Kesimpulan yang dapat diambil yakni kasein ÃŽÂ² susu kambing jika dicerna dengan enzim pencernaan dapat menghasilkan peptida bioaktif ACEi yakni INK.Identification of Angiotensin Converting Enzyme-inhibitor (ACEi) Bioactive Peptide from Goat Milk ÃŽÂ²-Casein with It's Polymorphism by In Silico TechniqueAbstractPolymorphism eventually may be occurred at the protein level. Changes in the amino acid sequence due to polymorphism may exhibit a potential action to generate of the angiotensin-converting enzyme inhibitors (ACEi) bioactive peptide. This study is aimed to assess bioactive peptides that have a great potent value as ACEi from goat ÃŽÂ² casein along with its polymorphism. The research was done by in silico technique on goat ÃŽÂ²-casein sequence and three-dimensional structure human testicular ACE. Peptide-cutting simulations with digestive enzymes (pepsin, trypsin and chymotrypsin), peptide properties review, then ligand-receptor docking simulations was applied in this research. Appearance of Lipinski's Rule of Five (Ro5), bioactivity and affinity energy were considered for selecting bioactive peptides. The results show that bioactive peptide found as INK (Ile-Asp-Lys) which had similar ability as lisinopril (energy affinity Ã¢Â€Â“8.2kcal/mol vs. Ã¢Â€Â“8.3kcal/mol). The INK peptides could be found from the hydrolysis resulted in alleles A, C, D and E, therefore polymorphism did not affect the differences of production of bioactive peptides. A conclusion, processed goat milk ÃŽÂ² casein with digestive enzymes could produce ACEi of INK as bioactive peptide.
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