ABSTRAK

Latar Belakang: Diabetes Melitus (DM) adalah penyakit metabolik yang prevalensinya terus meningkat tiap tahun di Indonesia. Pendekatan terapi yang umum digunakan melibatkan penghambatan enzim α-glukosidase. Sinamaldehid telah dikenal memiliki potensi antidiabetes dengan cara menghambat enzim α-glukosidase. Penelitian ini melibatkan turunan sinamaldehid, seperti α-bromosinamaldehid, α-klorosinamaldehid, α-α-metilsinamaldehid, asam sinamat, dan metil sinamat, yang memiliki struktur serupa.
Tujuan: Mengetahui potensi senyawa sinamaldehid dan turunannya sebagai inhibitor α-glukosidase dengan metode *docking* dan senyawa uji yang memiliki potensi aktivitas paling tinggi sebagai inhibitor α-glukosidase. Mengetahui toksisitas dari senyawa sinamaldehid, α-metilsinamaldehid, metil sinamat, asam sinamat, α-klorosinamaldehid, α-bromosinamaldehid.
Metode: Penelitian dilakukan dengan simulasi *docking* dan divisualisasikan dalam tingkatan molekuler secara 2D dan 3D serta dilanjutkan dengan pengujian tingkat toksisitas senyawa sinamaldehid dan turunannya menggunakan aplikasi berbasis *website* ProTox-II.
Hasil: Skor *docking* pada sinamaldehid, α-metilsinamaldehid, metil sinamat, asam sinamat, α-klorosinamaldehid, α-bromosinamaldehid berturut-turut adalah : -59,55 ; -54,41; -57,73; -59,94; -54,46; -54,45. Uji toksisitas menurut GHS berdasarkan nilai LD50 senyawa sinamaldehid, α-metilsinamaldehid, metil sinamat, asam sinamat, α-klorosinamaldehid, α-bromosinamaldehid berturut-turut termasuk ke dalam kelas 4 (1850mg/kgbb); 5(2050mg/kgbb); 5(2610mg/kgbb); 5(2500mg/kgbb); 5(2031mg/kgbb); 4(470mg/kgbb).
Kesimpulan: Senyawa sinamaldehid dan turunannya berpotensi menghambat alpha glucosidase. Hasil uji toksisitas dari sinamaldehid dan bromocinnamaldehyde berdasarkan GHS termasuk ke dalam kelas 4, sedangkan klorocinnamaldehyde, methylcinnamaldehyde, cinnamic acid, dan methyl cinnamate termasuk ke dalam kelas 5.

Kata Kunci: *alfa-glukosidase, molecular docking, acarbose, sinamaldehid*

ABSTRACT

Background: Diabetes Mellitus (DM) is a metabolic disease which prevalence's is increasing every year in Indonesia. A common therapeutic approach involves the inhibition of the α-glucosidase enzyme. Cinnamaldehyde is known to have antidiabetic potential by inhibiting the α-glucosidase enzyme. This study involves derivatives of cinnamaldehyde, such as α-bromocinnamaldehyde, α-klorocinnamaldehyde, α-methylcinnamaldehyde, Cinnamic acid, and Methyl cinnamate, which have similar structures.
Objective: To determine the potential of cinnamaldehyde and its derivatives as α-glucosidase inhibitors using *docking* methods and to identify the compound with the highest potential activity as an α-glucosidase inhibitor. To assess the toxicity of cinnamaldehyde, α-methylcinnamaldehyde, methyl cinnamate, cinnamic acid, klorocinnamaldehyde, and bromocinnamaldehyde.
Methods: The study was conducted through *docking* simulations, visualized at the molecular level in 2D and 3D, and followed by toxicity testing of cinnamaldehyde and its derivatives using the web-based ProTox-II application.
Results: The *docking* scores for cinnamaldehyde, α-methylcinnamaldehyde, methyl cinnamate, cinnamic acid, klorocinnamaldehyde, and bromocinnamaldehyde were, respectively: -59.55; -54.41; -57.73; -59.94; -54.46; -54.45. Toxicity tests according to the Globally Harmonized System (GHS) based on the LD50 values for cinnamaldehyde, α-methylcinnamaldehyde, methyl cinnamate, cinnamic acid, klorocinnamaldehyde, and bromocinnamaldehyde were classified as follows: Class 4 (1850 mg/kgbw); Class 5 (2050 mg/kgbw); Class 5 (2610 mg/kgbw); Class 5 (2500 mg/kgbw); Class 5 (2031 mg/kgbw); Class 4 (470 mg/kgbw).
Conclusion: Cinnamaldehyde and its derivatives have potential in inhibiting alpha-glucosidase. Toxicity test results for cinnamaldehyde and bromocinnamaldehyde based on the GHS classification fall into Class 4, while klorocinnamaldehyde, methylcinnamaldehyde, cinnamic acid, and methyl cinnamate fall into Class 5.

Keywords: *alpha-glucosidase, molecular docking, acarbose, cinnamaldehyde*