

## Analisis dinamika molekuler hasil penambahan kompleks $\alpha$ -glukosidase dengan sulokrin = Molecular dynamic analysis of docking product of complex $\alpha$ -glucosidase with sulochrin

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### Abstrak

Sulokrin telah dilaporkan memiliki aktivitas sebagai inhibitor  $\alpha$ -glukosidase. Model tiga dimensi (3D) enzim dikonstruksi berdasarkan struktur kristal  $\alpha$ -glukosidase *S. solphataricus* (MaA) dan sub-unit N-terminal Maltase-Glucoamilase manusia (NtMGAM) (Saqib & Siddiqi, 2008) menggunakan Modeller9.10.

Penambatan sulokrin dilakukan pada dua bentuk konformasi yakni berdasarkan energi terbaik dan kluster terbaik menggunakan Autodock4.2 dan hasilnya menunjukkan nilai G secara berturut-turut yakni -6,90; -6,44 kkal/mol dan  $K_i$  = 8,74; 19,13 M, sebagai kontrol inhibitor  $\alpha$ -glukosidase digunakan akarbose, miglitol, voglibose, dan salacinol dengan skor nilai G = -7,80; -7,60; -6,56 dan -4,25 kkal/mol, serta  $K_i$  = 2,12; 2,77; 15,75 dan 482,55 M. Interaksi sulokrin pada situs aktif  $\alpha$ -glukosidase manusia dipelajari melalui simulasi dinamika molekuler menggunakan AMBER dan menunjukkan adanya interaksi kuat dan stabil pada residu Asp587, dibandingkan dengan akarbose yang menunjukkan interaksi dengan residu Asp587, Asp398, Asp511, dan Phe 518, sedangkan voglibose menunjukkan interaksi dengan residu Asp398 dan Asp511.

.....Sulochrin has reported active as  $\alpha$ -glucosidase inhibitor. The three-dimensional (3D) model of enzyme is constructed based on the crystal structures of the *S. solphataricus*  $\alpha$ -glucosidase (MaA) and Human N-terminal subunit of Maltase-Glucoamylase (NtMGAM) (Saqib & Siddiqi, 2008) by using Modeller9.10 program. Docking of sulochrin performed on two conformational form based on the best energy and best cluster by using Autodock4.2 and the result showed G value = -6.90, -6.44 kcal/mol and  $K_i$  value = 8.74, 19.13 M, respectively, as a control of  $\alpha$ -glucosidase inhibitor is used acarbose, miglitol, voglibose, and salacinol with a score of G value = -7.80, -7.60, -6.56, -4.25 kcal/mol and  $K_i$  value = 2.12, 2.77, 15.75, 482.55 M, respectively. Interaction of sulochrin to active site of Human  $\alpha$ -glucosidase has been studied by molecular dynamic simulation using AMBER and showed a strong and stable interactions with Asp587 residue, in comparison with acarbose showed interactions with Asp587, Asp398, Asp511, and Phe 518, while voglibose showed interactions with Asp398 and Asp511.