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Molecular Dynamics Simulation of Bioactive Compounds from Moringa Oleifera Leaf Powder Extract as Antidiabetic by Inhibiting α -Amylase and α -Glucosidase Enzymes

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Abstract

Diabetes is a chronic disease that has caused around 6.7 million deaths a year or one death every 5 s. Diabetes therapy usually focuses on the insulin hormone. In fact, in addition to regulating carbohydrate metabolism by the insulin hormone, therapy can be done by inhibiting several enzymes such as α -amylase and α -glucosidase in the starch and glycogen metabolism pathway as a source of blood glucose. This study investigates Moringa oleifera leaf powder (MOLP) from different Leaf stalk colors were screened for their inhibitory action of α -amylase and α -glucosidase against type 2 diabetes through molecular docking, molecular dynamics simulation, and in vitro enzyme inhibition. Rutin showed the highest binding affinity among 57 tested compounds. This compound

simultaneously binds to the 2 target proteins of α -amylase and α -glucosidase, with higher binding affinity values of -6.752 mol^{-1} for α -amylase and -8.756 mol^{-1} for α -glucosidase. The rutin glucosidase revealed to be the most stable molecule with the highest binding free energy through molecular dynamics simulation was MM-GBSA Binding Energy = $-33.3645 \pm 5.0338 \text{ kcal mol}^{-1}$ and MM-PBSA Binding Energy = $1.8598 \pm 5.5359 \text{ kcal mol}^{-1}$, indicating that it could compete with the inhibitor native ligand. The α -glucosidase inhibitory activity of the ethyl acetate extract achieved 81.58% inhibition, while acarbose achieved 84.47%. Rutin has the best potential as an inhibitor of the α -glucosidase enzyme and the stability of its interaction compared to other flavonoid groups, making it a prospective drug candidate for type 2 diabetes. © 2026, Walailak University. All rights reserved.

Author keywords

Diabetes mellitus; In silico; In vitro; Moringa oleifera; α -amylase; α -glucosidase

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Abstract

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