CONDEQUI
Congresso Online Nacional de Química

IN SILICO PREDICTION BY MOLECULAR DOCKING OF THE ANTIDIABETIC ACTIVITY OF ANTHOCYANIN-DERIVED COMPOUNDS FROM BANANA INFLORESCENCE (MUSA SPP.) TARGETING THE MALTASE-GLUCOAMYLASE ENZYME

VII Congresso Online Nacional de Química, 7ª edição, de 23/06/2025 a 25/06/2025
ISBN dos Anais: 978-65-5465-148-6

SILVA; João Paulo Souza Simão da [1], FERNANDES; Mirian Bomfim [2], JESUS; Jociel Honorato de [3], TRISTÃO; Taline Canto [4]

RESUMO

Compounds derived from the Musaceae family, specifically from the banana inflorescence (*Musa spp.*), have shown promising potential as antidiabetic agents. Previous studies have highlighted the effectiveness of bracts, rich in anthocyanins, in reducing glucose levels. This research aims to predict, through molecular docking computational simulation, the inhibitory potential of anthocyanin derivatives isolated from the banana inflorescence as candidates for maltase-glucoamylase (MGAM) inhibition. A quantitative-descriptive methodology was adopted to explore the interaction between the anthocyanin derivatives and MGAM. The *Protein Data Bank* (PDB) was used to select the target protein, and *PubChem* provided the chemical structures of the anthocyanin derivatives. The protein was retrieved using the identifier 2QMJ and prepared using *Biovia Discovery Studio software*, where the co-crystallized ligand and water molecules were removed. The active site was defined based on the coordinates provided in the protein file (x = -20.807977, y = -6.586273, z = -5.073705). These coordinates were used for both redocking and docking simulations. The molecular docking simulations were performed using *AutoDock Vina*, and the conformations with the lowest binding energies were selected for detailed analysis. Following validation of the molecular docking protocol (RMSD of 0.84 Å), the method was applied to evaluate the interaction of six anthocyanin derivatives with MGAM. The redocking of the co-crystallized ligand resulted in a binding energy of -8.10 kcal/mol, serving as a reference for comparative analysis. The binding energies obtained for the tested anthocyanin derivatives ranged from -8.8 to -9.3 kcal/mol, demonstrating higher affinity than the native ligand. Pelargonidin-3-rutinoside stood out with the lowest binding energy (-9.3 kcal/mol), suggesting a stronger interaction with MGAM. All analyzed molecules exhibited high affinity for the target protein, with subtle differences in their molecular interactions. Notably, the amino acids Glu658, Glu767, and Arg647 were consistently involved in hydrogen bonding interactions. Frequent interactions with Pro676 were also observed, a relevant aspect that could be decisive for drug design and for understanding the binding mechanism of these molecules. On the other

[1] Universidade Federal de Juiz de Fora - UFJF
[2] Universidade Federal de Juiz de Fora - UFJF
[3] Centro Universitário Faema - UNIFAEMA
[4] Centro Universitário Faema - UNIFAEMA

hand, no direct interactions were observed between the tested ligands and the main catalytic residues of the enzyme (His600, Asp327, Asp542, Arg526, and Asp203), suggesting that these compounds may act in regions adjacent to the catalytic site, possibly through allosteric mechanisms or steric hindrance. This study enhances the understanding of the therapeutic potential of anthocyanins derived from banana inflorescence (*Musa spp*.) in modulating MGAM, a relevant target for interventions in type 2 diabetes mellitus. Through molecular docking approaches, the compounds demonstrated promising affinity for the enzyme, supporting the continuation of investigations into anthocyanins as antidiabetic agents.

PALAVRAS-CHAVE: Molecular Docking, Anthocyanins, Maltase-Glucoamylase (MGAM)

[1] Universidade Federal de Juiz de Fora - UFJF
[2] Universidade Federal de Juiz de Fora - UFJF
[3] Centro Universitário Faema - UNIFAEMA
[4] Centro Universitário Faema - UNIFAEMA