OSP-02

Unlocking the Antidiabetic Potential of Anthraquinones: *In Silico* Docking Insights Against α-Amylase and α-Glucosidase

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Diabetes mellitus (DM) is a major global health concern, characterised by impaired glucose regulation and postprandial hyperglycaemia. Current therapeutic options, such as acarbose, an α-amylase and α-glucosidase inhibitor, are effective but often associated with gastrointestinal side effects. This has prompted the search for safer alternatives with comparable efficacy. Anthraquinone derivatives, known for their diverse biological activities, represent promising scaffolds for the development of novel enzyme inhibitors. In this study, fourteen anthraquinone derivatives (AQ1–AQ14) were evaluated using molecular docking to assess their inhibitory potential against α-amylase (PDB: 1B2Y) and α-glucosidase (PDB: 5NN8). Docking simulations were performed in AutoDock Vina, and visualisation of binding interactions was carried out using Discovery Studio Visualizer. All tested compounds demonstrated binding energies comparable to acarbose, suggesting strong inhibitory potential. AQ12 and AQ13 exhibited the highest affinity for α-amylase, while AQ8 and AQ14 bound most strongly to α-glucosidase. AQ14, in particular, formed the greatest number of hydrophobic interactions, contributing to enhanced binding stability. Key catalytic residues, including His305 in α-amylase and Asp518 in α-glucosidase, were effectively targeted by several derivatives, supporting their inhibitory activity. Based on docking scores and interaction profiles, AQ7, AQ9, and AQ12 emerged as the most promising candidates, displaying strong inhibitory potential against both enzymes. These findings provide compelling *in silico* evidence that anthraquinone scaffolds could serve as effective alternatives to acarbose. Further experimental validation is warranted to confirm their enzyme inhibitory activities and therapeutic potential in managing postprandial hyperglycaemia.

Keywords: Aromatic organic compounds, Binding affinity, Hyperglycaemia, Molecular docking, Quinones

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