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In silico comparative analysis of curcumin and acarbose as inhibitors of human pancreatic alpha-amylase

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Human pancreatic α-amylase is an important therapeutic target for drug development to control postprandial blood glucose levels in Type 2 Diabetes Mellitus (T2DM). Curcumin, the main bioactive polyphenol of *Curcuma longa* (turmeric), was investigated for its ability to inhibit human pancreatic α-amylase through *in silico* molecular docking studies (PDB ID: 1B2Y; 1.50 Å resolution). Molecular docking simulations were carried out using the AutoDock Vina software to investigate the binding affinity and interaction profile of curcumin in the catalytic active region of the enzyme. From docking studies, it was revealed that the interactions of curcumin with key catalytic residues Asp197, Glu233, and Asp300, which are directly involved in the cleavage of the glycosidic bond, occur within the deep catalytic pocket of α-amylase. Curcumin showed binding strength similar to that of the common α-amylase inhibitor, acarbose, with a binding affinity of −7.3 kcal/mol. The interaction studies showed that the localized hydrogen bonding, hydrophobic contacts, and π-related interactions (π − σ and π-alkyl interactions with ILE396, VAL452 residues) favour the stability of the curcumin-enzyme complex. However, acarbose formed a wide network of hydrogen bonds with residues such as GLU438 and ARG10. Computational data suggest that curcumin has useful structural and physicochemical properties that allow it to interact with the catalytic region of human pancreatic α-amylase. Furthermore, this study highlights the importance of traditional medicinal plants like *Curcuma longa* in modern drug development research. The results indicate that curcumin may be a potential natural candidate for the development of anti-diabetic drugs for the future targeting postprandial hyperglycemia.

Keywords:

Alpha-amylase, Curcumin, Molecular Docking, Type 2 Diabetes, Ethnopharmacology

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