Computational drug design of potential α-amylase inhibitors using some commercially available flavonoids

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Abstract:

Diabetes mellitus is turning out to be the most common chronic disease and the affected population and its significantly increasing. Flavonoids are a group of natural products which exhibits various biological and pharmacological activities. The primary objective of this study was to investigate the α-amylase inhibitory activity of flavonoids using *in silico* docking studies. In this perspective, flavonoids like biochanin, chrysin, hesperitin, morin, tricin and vitexycarpin were selected. Acarbose, a known α-amylase inhibitor was used as the standard. *In silico* docking studies were carried out using AutoDock 4.2, based on the Lamarckian genetic algorithm principle. The interacting residues within the complex model and their contact types were identified. In the docking studies, three important parameters like binding energy, inhibition constant and intermolecular energy were determined. The results showed that all the selected flavonoids showed binding energy ranging between -7.20 kcal/mol to -6.21 kcal/mol when compared with that of the standard (-2.94 kcal/mol). Inhibition constant (5.31 µM to 27.89 µM) and intermolecular energy (-8.99 kcal/mol to -7.41 kcal/mol) of the flavonoids also coincide with the binding energy. All the selected flavonoids contributed α-amylase inhibitory activity because of its structural properties. The α-amylase inhibitory activity of the selected flavonoids was in order of tricin>hesperitin>vitexycarpin>chrysin>morin>biochanin. These molecular docking analyses could lead to the further development of potent α-amylase inhibitors for the treatment of diabetes. Further investigations on the above compounds and *in vivo* studies are necessary to develop potential chemical entities for the prevention and treatment of diabetes.