عنوان مقاله:

Identification of Potential Glucosyltransferase Inhibitors from Cinnamic Acid Derivatives Using Molecular Docking Analysis: A Bioinformatics Study

محل انتشار:

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خلاصه مقاله:

Background: Dental caries is one of the most common oral chronic diseases. Streptococcus mutans is the mainpathogenic bacteria playing a role in degrading the mineral texture of the teeth. Glucosyltransferase (GTFase)of S. mutans is responsible for producing glucan, which is the main exopolysaccharide found in the cariogenicbiofilms. Further, previous studies have reported that cinnamic acid diminished biofilm formation of S. mutans.Therefore, we hypothesized that cinnamic acid and its derivatives might act as GTFase inhibitors.Methods: The binding affinity of a total of ۱۲ plant-based compounds including cinnamic acid and its ۱۱derivatives to the GTFase active site were examined by utilizing the AutoDock tool. The possible interactionsbetween top-ranked cinnamic acid derivatives and the residues within the GTFase catalytic site were also takeninto consideration.Results: Five of the cinnamic acid derivatives including rosmarinic acid (RA), cynarine, chlorogenic acid (CGA),caffeic acid ۳-glucoside, and N-p-coumaroyltyramine demonstrated inhibitory effects on GTFase at nanomolarconcentration. Stabilizing interactions such as π–π stack pairing and pi-charge interactions were detectedbetween top-ranked GTFase inhibitors and residues within the enzyme active site.Conclusions: The present study suggests that RA, cynarine, CGA, caffeic acid ۳-glucoside, and N-pcoumaroyltyraminemight have protective effects on dental caries, and therefore, may be considered as antitoothcaries compounds.

کلمات کلیدی:

Cinnamic acid, Dental caries, Glucosyltransferase, Inhibitor, Molecular docking