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A Molecular Docking Study on Anticariogenic Properties of Theaflavins against *Streptococcus mutans*

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Abstract Early childhood caries (ECC) is an aggressive manifestation of dental decay, linked to high levels of *Streptococcus mutans* in dental plaque. In Malaysia, over 70% of children suffer from ECC, leading to premature tooth loss, malnutrition, and reduced quality of life. Common dental-care ingredients like triclosan and triclocarban pose health risks, necessitating safer alternatives. Theaflavins, bioactive compounds in black tea, show potential as natural antimicrobial agents. However, the precise molecular interactions of theaflavins with key virulence-associated proteins

of *S. mutans* remain underexplored. This study aims to investigate the antibacterial mechanisms of theaflavins against *S. mutans* using in-silico methods. PyRx was used to evaluate the binding affinities of four selected compounds, theaflavin (TF1), theaflavin-3gallate (TF2A), theaflavin-3'-gallate (TF2B), and theaflavin-3,3'-digallate (TF3), against seven *S. mutans* proteins (PDB 4TQX: Sortase A, PDB 6CAM: Glucan binding protein, PDB 3QE5: Cell surface protein, PDB 3VX4: Quorum sensing, PDB 3AIC: Glucosyltransferase, PDB 2W3Z: Immune evasion, PDB 3CZC: Carbohydrate uptake). All the ligands were prepared and optimised using Avogadro-1.2 prior to the molecular docking. BIOVIA Discovery visualizer was used to observe the protein-ligand interactions. Findings indicated that theaflavins exhibit significant binding affinities to various *S. mutans* proteins. Among all tested compounds, TF3 demonstrated the strongest binding affinities and favourable hydrogen bonding, particularly against glucan binding protein and glucosyltransferase. These results suggest that TF3 may serve as a promising mechanisms.

Keywords

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