# ABSTRACT

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**_IN SILICO_ STUDY OF BETEL (_Piper betle_ L.) LEAVES ACTIVE COMPOUNDS AS INHIBITORS AGAINST _Streptococcus mutans_**
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(xi + 36 pages, 6 tables, 16 figures, 1 appendix)

Dental caries is an oral disease resulting from teeth demineralization in an acidic environment, with *Streptococcus mutans* being the major pathogen. Synthetic microbial agents are often used for caries treatment. However, due to the undesirable side effects, there has been a shift in interest to discover natural anticariogenic agents which can be incorporated in food product. Betel (*Piper betle* L.) leaves are medicinal plants containing various active compounds. *In vitro* studies demonstrated the potential of betel leaves extracts in inhibiting *S. mutans* growth and biofilm formation. The objective of this research was to conduct *in silico* study of betel leaves active compounds as inhibitors against *Streptococcus mutans*. This study was conducted using computer hardware and softwares. Ligand and protein preparation were conducted using Open Babel GUI 3.1.1 and PyMOL 2.5.2. Molecular docking was conducted using PyRx-Python 0.8 – Autodock Vina after method validation. Visualization was performed in 2D using BIOVIA Discovery Studio 2021 and 3D using PyMOL 2.5.2. Target proteins selected from *S. mutans* were glucan-binding protein C and antigen I/II carboxy-terminus. Betel leaves active compounds chosen as test ligands were obtained from GC-MS chromatograms of its ethanolic extract. Selected ligands toward GbpC were α-cadinene, α-selinene, α-cubebene and β-selinene. Selected ligands toward Ag I/II carboxy-terminus were β-selinene, α-selinene, α-cadinene and caryophyllene. Visualization of protein-ligand interaction revealed that test ligands bind with residue Val410 from GbpC and residues Lys1032, Ala1034, and Tyr1105 from Ag I/II carboxy-terminus, which have been previously identified to play role in pathogenesis of dental caries by *S. mutans.*

Keywords : Betel (*Piper betle* L.) leaves, *Streptococcus mutans*, glucan-binding protein C, antigen I/II, molecular docking
Reference : 49 (2011-2021)