



**AN *INSILICO* STUDY OF QUINIC ACID DERIVATIVES AS INHIBITORS OF COM
A, THE QUORUM SENSING PROTEIN OF *STREPTOCOCCUS MUTANS*
RESPONSIBLE FOR THE PATHOGENESIS IN DENTAL CARIES**

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ABSTRACT

Dental caries is considered to be one of the important infectious diseases throughout the world. It was recognized that the *Streptococcus mutans*, plays an important role in cariogenesis. The oral streptococci in biofilms may communicate by a quorum-sensing CSP signalling system. The products of at least six genes, *comAB*, *comX*, and *comCDE*, are involved in CSP signalling. It has been proved that loss of Com A attenuates the formation of biofilm. In the present study quinic acid derivatives have been developed *insilico* as the inhibitors of Com A and a molecular docking study is performed to find its efficiency as inhibitors. The three dimensional structure of Com A was retrieved from RCSB- PDB database. The possible binding sites of Com A were searched using binding site prediction 3DLIGANDSITE. The structure of quinic acid was obtained from ZINC database. A total of 100 ligands were generated with the help of software ACD chemsketch. Rapid virtual screenings of these compounds were performed in the docking tool iGEMDOCK v2.0. Based on the binding energy a total of five ligands were selected for the further study. The selected five ligands were then analyzed for drug- relevant properties based on “Lipinski’s rule of five” and other drug like properties. The docking of five ligands was performed using AutoDock 4.0 software. From the present study, it has been found that (1R)-1, 3, 4-trihydroxy-5-methylcyclohexane carboxylic acid, which is a novel compound, a derivative of quinic acid, can act has an inhibitor for the Com A.

**Keywords: *Streptococcus mutans*, Dental Caries, Com A, Quinic Acid Derivatives and
Molecular Docking**