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## **P177 - Molecular docking analysis of Sortase A from Streptococcus mutans reveals spontaneous interaction with flavonoid chalcone**

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**Short Abstract:** Background: Human dental caries is considered a globally important disease, which is associated with the progressive loss of teeth. This process begins with the formation of bacterial biofilms by Streptococcus mutans which causes teeth demineralization and other related diseases. Between main virulence factors, sortase A (SrtA) is involved in the adhesion of bacterial surface proteins to promote biofilm formation. In the present work, a molecular docking evaluation was performed to determine specific interaction between SrtA and chalcone.

Results: Protein sequence for wild type SrtA from S. mutans (Q8CM62) was obtained and conserved residues, as well as homology modelling, were analyzed. Furthermore, molecular docking and protein interaction networks were determined using SwissDock and STRING. For phylogenetic analysis, G-INS-1 method and MAFFT 7 interface were used. After multiple alignment analysis, catalytic triad formed by Cys205, His139 and Arg213 was found, which shows a high conservation between other sortases. Based on different enzyme-inhibitor templates obtained by molecular docking, the result with the lowest energy was chosen ( $\Delta G = -5.12$ ) which shows that interaction between SrtA and chalcone was spontaneous. Between different proteins involved in the same network as SrtA, values of 50.3% and 66.2% were obtained for *gyrA* and *ldh*, respectively. Finally, the G-INS-1 phylogenetic tree shows a high conservation of these enzymes in Gram-positive bacteria.

Conclusion: Sortase A from Streptococcus mutans is a basic molecule that specifically interacts with flavonoid chalcone, which is considered of medical relevance for oral health.

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