Molecular docking of glucosyltransferase enzyme (The most important factor in development of dental plaque) with *Myrtus* compounds

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Abstract: Glucosyltransferase from *Stereptococcus mutans* (The most famous bacterium which play a key roll in dental decay) is one of the most important factors in development of dental plaque. A recent experimental study has shown blocking effect of *Myrtus* extract on glucosyltransferase activity. Aim of this study was to recognize the most effective compound in the plant extract. To achive this goal we used molecular docking. Molecular docking is a valuable method to recognize ligand-receptor interactions. We can understand blocking activity of compounds from these interactions. First of all, structures of six major compounds (compounds which constitute more than 2% of the *Myrtle* extract) and penicillin as positive control was obtained from PubChem database and then converted to MOL format by Open Bable software. After that, sequence of one of the eight similar chains of the protein was obtained from NCBI database and 3-D structure was predicted by Swiss Model server. Then Autodock was used to prepare the protein molecule for docking. After all, iGemdock was used for docking. Result of this study shoed different levels of blocking activity among the compounds. The most effective compound was 1,8 cineole which constitute 28% of oil extract of *Myrtus*. The compound was as effective as penicillin compairing fitness numbers.

Keywords: Docking; *Stereptococcus mutans*; Glucosyltransferase ; *Myrtus*; Dental decay

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