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Biophysical Mechanics of the Dental Bacteria Biofilm and Polyphenols as Reactive Oxygen Species Reducers

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Abstract

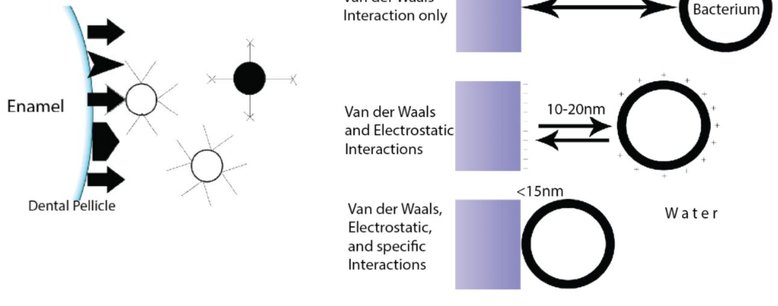
Biofilms are thin layers that consist of colonies of bacteria. These biofilms are full of matrices of extracellular polymeric substance. Biofilms specifically formed by pathogenic Gram-negative Escherichia coli strains are often resistant to antimicrobial agents and they can be truly deleterious to dental structures causing infections. Accumulation of various bacteria that forms dental plaque causes the periodontal disease. Diffusing through a pellicle and adaptive interactions of the microbial molecules with the microorganisms make them resistant to antimicrobial agents. In this research, molecular mechanisms of the process were studied through computational simulations. Computational modeling was employed to find the electrostatic and hydrophobic interaction of a component of a bacterial protein's side chain and a component of the acquired pellicle. In addition, polyphenols, which inhibit the formation of plaque caused by the Streptococcus mutans, were computationally model
ed and biochemically analyzed to find their bond properties and enthalpy of formations.

Introduction

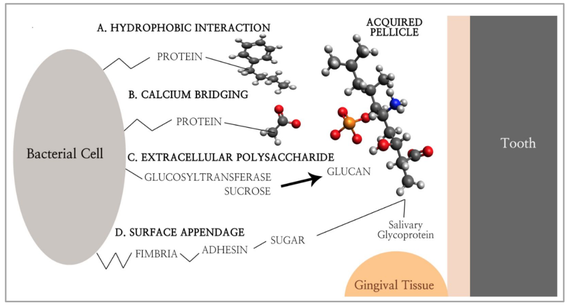
Biofilms are thin layers that consist of colonies of bacteria. These biofilms are full of matrix of extracellular polymeric substance. Biofilms specifically formed by pathogenic Gram-negative Escherichia coli strains can be truly deleterious to humans, causing prostatitis, biliary tract infections, and urinary catheter cystitis. These bacteria are often resistant to antimicrobial agents, and their existence on medical devices are threatening to humans. *Aronia melanocarpa,* commonly known as black chokeberry, is often considered as the healthiest fruit known to man. Named as a super food, Aronia brings many health benefits from its anti-carcinogenic and anti-inflammatory properties. Aronia is an antioxidant and helps people with heart disease recovery, weightloss, and urinary track health. *Aronia melanocarpa* may have further, more important health benefits. This study examines Aronia extracts, subfractions, and compounds, to determine the ability of Aronia in preventing biofilm formation and inhibiting bacterial growth.

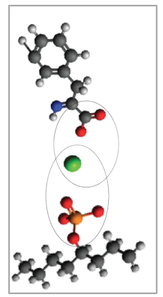
Bacterial Film & Dental Plaque

The remains of the reduced enamel epithelium after a tooth emerges into the oral cavity are worn off and digested by salivary and bacterial enzymes. When a tooth eruption occurs, that tooth is immediately covered by a thin and miniscule coating of saliva material also known as a pellicle. The pellicle is exogenous, since it is produced and obtained after the tooth eruption occurs. It is not produced during the development of teeth but formed by a substance from outside the tooth. The bacteria from your mouth tend to build colonies in the pellicle.



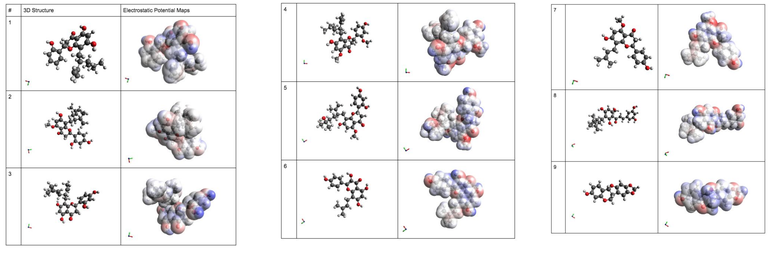
Dental Plaque Formation

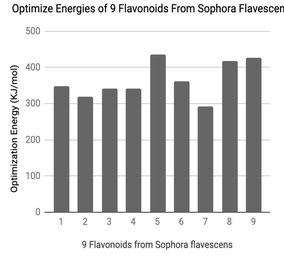


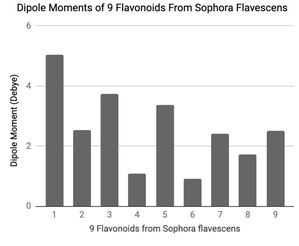


The beginning of plaque formation takes around two hours. Colonization involves growing of several isolated colonies, often restricted to microscopic tooth surface irregularities. The bacteria start to multiply and the colony starts to grow bigger from the nutrients from saliva and host foods. After about 21 days, the growth rate slows down and the plaque growth becomes stable. These colonies are rapidly and constantly covered by saliva.

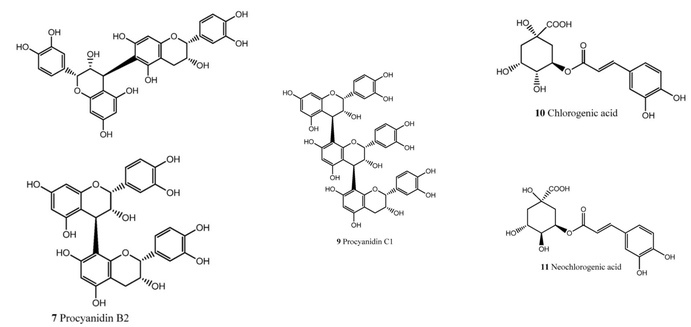
Polyphenol - Molecular Mechanisms



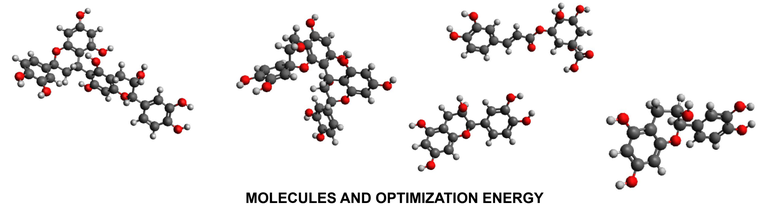




Data Analysis

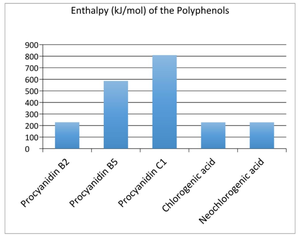


PHENOL MOLECULES



MOLECULES AND OPTIMIZATION ENERGY

Previous research on controlling biofilm infections included the effect of cranberry extracts on oral biofilms, biofilms produced on contact lenses, and biofilms produced by E. coli strains. The studies concluded that cranberry juice can lead to a decrease in pathogenic bacteria's ability to develop biofilm, perhaps because cranberry contains A-type proanthocyanidins, active constituents that prevent the attachment of bacteria.



Conclusion

In this research, a computational modeling was employed to find the electrostatic and hydrophobic interaction of a component of bacterial protein's side chain and a component of the acquired pellicle. In addition, polyphenols, which inhibit the formation of plaque caused by the Streptococcus mutans, were computationally modeled and biochemically analyzed to find their bond properties and enthalpy of formations.