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Photosynthetic pigment on dental health: An *in silico* approach

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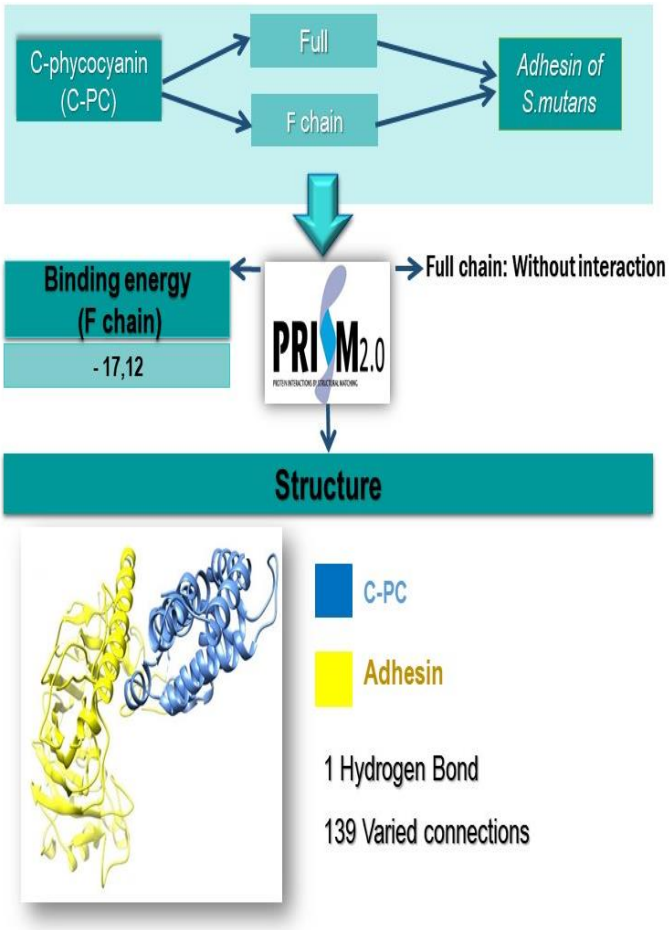
Graphical Abstract



Abstract.

The Streptococcus mutans is one of the main etiologic agents of multifactorial disease of caries. Adhesins like the antigen I / II are proteins of S. mutans and play an important role in caries lesions, even being a target for anti-cavity vaccines. C-phycocyanin (C-PC) is a blue-green heteroprotein which acts as a photosynthetic pigment for cyanobacteria such as Spirulina (Arthrospira) platensis and it has antibacterial effects. Thus, the C-PC could block the adhesins and represent an inhibition the caries process. Verifying the possible docking beween C-PC and adhesion protein antigen I/II of S. mutans in the main goal of this study. We used the PRISM web server (algorithm based on structural matching) for to check the interaction of the C-PC in its complete form (Full) or F chain with adhesion protein (antigen I / II) of S. mutans. The Full C-PC did not interact with the adhesion, while the F chain interacted with a binding energy of -17.12 establishing 01 Hydrogen bond and 139 varied connections (polar, nonpolar, favorable and unfavorable). Thus, the interaction of F chain with adhesion protein of S. mutans indicates a possible anticaries role of C-PC, encouraging continuity of studies in this area.

Introduction

S. mutans, a Gram-positive bacteria, is the major etiological agent of human dental caries and lives primarily in biofilms on the tooth surfaces. S. mutans possesses multiple high-affinity surface adhesins that enable colonization of the oral cavity. The Antigen I/II is one of the most widely studied adhesins and mediates bacterial attachment to the tooth's salivary pellicle, being fundamental for the establishment of caries (1,2). *So, the loss of adhesin function could prevent the formation of cavities. In this context, appear the alternative of using C-phycocyanin (C-PC). C-PC is a blue-green heteroprotein which acts as a photosynthetic pigment for cyanobacteria such as Spirulina (Arthrospira) platensis* (3) *which could interfere with the functionality of adhesins. Considering C-PC in preventing caries is possible for two main reasons: its previously reported antimicrobial action* (4) *and your security because the S. platensis, one of the main sources of C-PC, has GRAS status (Generally Recognized As Safe) issued by Food and Drug Administration (FDA)* (5). *Therefore, the objective of this study was to verify, through molecular docking, the interaction of C-PC with Antigen I/II of S. mutans for to predict possible capacity of C-PC inhibit adhesins and prevent caries.*

Materials and Methods

Proteins structures were obtained from Protein Data Bank (PDB) (6) *according PDB ID. For protein interaction verification we used the PRISM web server, (available on http://cosbi.ku.edu.tr/prism/) considering C-PC (PDB ID: 1GH0, in full structure or F chain only) and V-region of antigen I/II of S. mutans (adhesion; PDB ID 1JMM). The adhesion was subjected to docking simulation with: 1- C-PC full structure and 2- only F chain totaling 2 docking simulations (we provided on the server PDB ID for each pair of proteins). The possible binding modes were generated by server (number of possible binding modes depending of pair analyzed) and only the most negative binding energy (greater stability) was showed in results. The binding mode with greater binding energy was analyzed with UCSF Chimera program (available to download at http://www.cgl.ucsf.edu/chimera/download.html).for verification of Hydrogen bonds and varied connections (polar, nonpolar, favorable and unfavorable) established between molecules.*

Results and Discussion

The Full C-PC did not interact with the adhesion, while the F chain interacted with a binding energy of -17.12 establishing 01 Hydrogen bond and 139 varied connections (polar, nonpolar, favorable and unfavorable). The full C-PC structure is extremely large (110 Å diameter) (7) what should prevent its biological action. The F chain, on the other hand, is smaller and had already demonstrated a biological action in a previous study (8). *The interaction of the F chain with adhesin demonstrates an anti-caries potential of C-PC, however, in vitro and in vivo studies are needed to verify whether this interaction translates into a biological effect to reduce caries.*

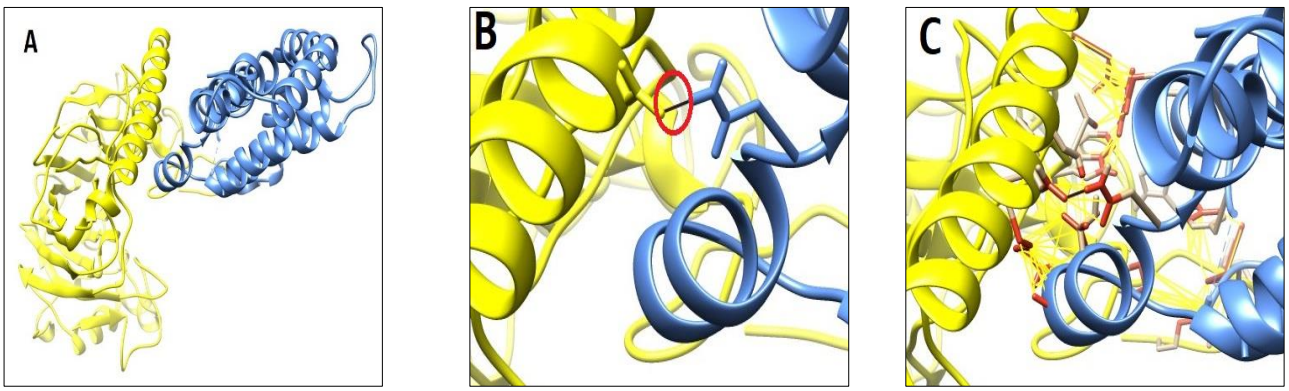


Figure 1: F chain of C-phycocyanin (C-PC) (blue) and V-region of antigen I/II of Streptococcus mutans (adhesin) (yellow) (A). Hydrogen bonds between F chain and adhesin (black stroke with red circle around) (B). Varied connections (polar, nonpolar, favorable and unfavorable) between F chain and adhesin (yellow strokes) (C).

Conclusions

The interaction of F chain with adhesion protein of S. mutans indicates a possible anticaries role of C-PC, encouraging continuity of studies in this area.

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