

Conformational Analysis of the Human Salivary Protein IB7₁₄ Complexed with Procyanidin B3 Tannin Molecules

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The protein fragment IB7₁₄ contains fourteen amino acids (SPPGKPQGPPQGG) of the intrinsically unstructured human salivary protein IB7, which has the ability to non-covalently bind to procyanidin tannin molecules. In addition to a number of foods, tannin molecules are most commonly found in red wines. When the tannins complex with the IB7, the dry-mouth feeling known as astringency is observed due to the precipitation of the previously lubricating salivary proteins. The goal of this research is to characterize this complexation and analyze the conformational changes between the uncomplexed and complexed IB7₁₄ salivary proteins. To conduct this analysis, we are using conformational data created from Monte Carlo simulations of both the simplified uncomplexed IB7₁₄ and the protein complexed with model tannins (see Figure 1 and Figure 2). These data are clustered using self-organizing maps (SOM) in order to classify the conformations of the IB7₁₄-tannin complexes in relation to the uncomplexed protein. Previous NMR studies coupled with molecular modelling have found that there is little to no change in the secondary structure of the intrinsically unstructured protein upon complexation. However, it was shown that there is a decrease in the conformational disorder of the protein. Our preliminary results suggest that the presence of tannins does not induce novel conformations of the IB7₁₄ salivary protein. Furthermore, it appears as though the conformational distribution is less broad for the complexed IB7₁₄ compared to the uncomplexed protein, which is consistent with the above experimental results.

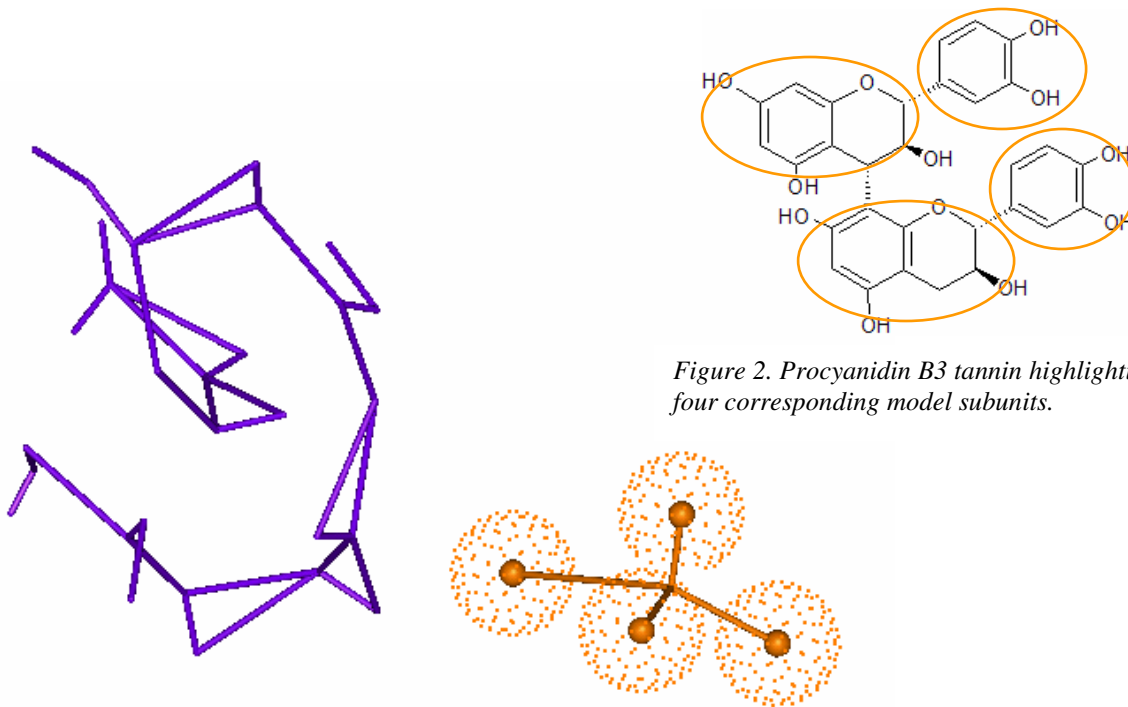


Figure 1. A simplified model of salivary protein IB7₁₄ (purple) complexed with a model four subunit tannin molecule (yellow).

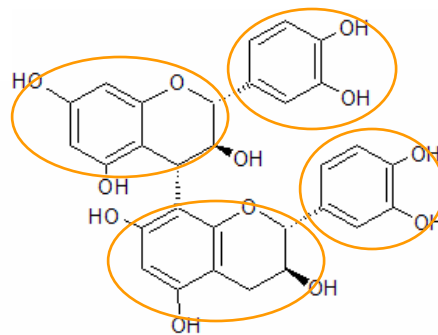


Figure 2. Procyanidin B3 tannin highlighting the four corresponding model subunits.