

## Conformational Analysis of the Human Salivary Protein IB7<sub>14</sub> Complexed with Procyanidin B3 Tannin Molecules

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The IB7<sub>14</sub> is a fourteen amino acid segment of the IB7 protein, which is found in saliva. It has the capability of binding non-covalently to tannin molecules which are found in various foods and wines, giving a rough, dry feeling in the mouth (astringency). The goal of this research is to characterize this binding and analyze the conformational changes of the protein during these interactions. We are using Grand Canonical Monte Carlo simulations of the IB7<sub>14</sub> fragment along with multiple tannin molecules. Two dimensional NMR results have shown that the IB7<sub>14</sub> fragment is much more restricted in its conformational diversity in the presence of tannins than in the absence of tannins. We are using a simplified model to simulate this system (see Figure below). We hope to closely reproduce the experimental results with respect to conformational diversity and tannin to protein interactions.

