

## **Intrinsic Disorder in the Human Salivary Protein Fragment IB7<sub>14</sub>**

Bryan VanSchouwen, Heather L. Gordon

*Department of Chemistry and Center for Biotechnology, Brock University,  
St. Catharines, ON, Canada, L2S 3A1*

**IB7<sub>14</sub>** is the 14-residue amino-terminal fragment of **IB7**, a human salivary protein whose function is to bind polyphenol molecules, known as **tannins**, found in certain foods and beverages. In the current work, intrinsic disorder within the human salivary protein fragment IB7<sub>14</sub> is being studied, and the structural nature of the binding of IB7<sub>14</sub> to the red wine tannin **procyanidin B3** is being investigated. IB7<sub>14</sub> is believed to exist in an extended and very dynamic structure, whose secondary structure consists of two polyproline II helices separated by a flexible Glycine rotula.<sup>1</sup> Previous solution-phase 2D NMR experiments have shown that three tannin molecules can bind to one IB7<sub>14</sub> molecule, with the result of a reduction in the structural flexibility of the IB7<sub>14</sub>.<sup>1</sup>

First, a series of independent Metropolis Monte Carlo (MMC) simulations of IB7<sub>14</sub> in the absence of procyanidin B3 have been performed, in order to examine the ensemble of 3D structures exhibited by the IB7<sub>14</sub>. Now, a series of independent Grand Canonical Monte Carlo (GCMC) simulations of IB7<sub>14</sub> in the presence of procyanidin B3 are being performed, in order to study the IB7<sub>14</sub>-tannin binding. The results of the two sets of simulations are being analyzed by various conformational analysis methods, including root-mean-square distance (RMSD) and end-to-end distance measurements. Finally, the two sets of results are being compared in order to assess the structural nature of IB7<sub>14</sub>-tannin binding, and the effect of this binding on the structural ensemble exhibited by IB7<sub>14</sub>.

- (1) Simon, C., Barathieu, K., Laguerre, M., Schmitter, J.M., Fouquet, E., Pianet, I., and Dufourc, E.J. "Three-Dimensional Structure and Dynamics of Wine Tannin-Saliva Protein Complexes. A Multitechnique Approach." *Biochemistry* **2003**, *42*, 10385-10395.