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Effect of Natural Molecular Crowding on the Structure and Stability of DNA Duplex

Authors : Chaudhari S. G., Saxena, S.

Abstract : We systematically and quantitatively investigated the effect of glucose as a model of natural molecular crowding agent on the structure and thermodynamics of Watson-Crick base paired three duplexes (named as D1, D2 and D3) of different base compositions and lengths. Structural analyses demonstrated that duplexes (D1 and D2) folded into B-form with different cations in the absence and presence of glucose while duplex (D3) folded into mixed A and B-form. Moreover, we demonstrated that the duplex was more stable in the absence of glucose, and marginally destabilized in its presence because glucose act as a weak structure breaker on the tetrahedral network of water. In the absence of glucose, the values of ΔG°25 for duplex (D1) were -13.56, -13.76, -12.46, and -12.36 kcal/mol, for duplex (D2) were -13.64, -12.93, -12.86, and -12.30 kcal/mol, for duplex (D3) were -10.05, -11.76, -9.91, -9.70 kcal/mol in the presence of Na+, K+, Na+ + Mg++ and K+ + Mg++ respectively. At high concentration of glucose (1:10000), there was increase in ΔG°25 for duplex (D1) -12.47, -12.37, -11.96, -11.55 kcal/mol, for duplex (D2) -12.37, -11.47, -11.98, -11.01 kcal/mol and for duplex (D3) -8.47, -9.17, -9.16, -8.66 kcal/mol. Our results provide the information that structure and stability of DNA duplex depends on the structure of molecular crowding agent present in its close vicinity. In this study, I have taken the hydration of simple sugar as an essential model for understanding interactions between hydrophilic groups and interfacial water molecules and its effect on hydrogen bonded DNA duplexes. On the basis of these relatively simple building blocks I hope to gain some insights for understanding more generally the properties of sugar–water–salt systems with DNA duplexes.

Keywords : natural molecular crowding, DNA Duplex, structure of DNA, bioengineering and life sciences
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