Entropy Calculations of Hybrid Nucleic Acid Systems

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Molecular dynamics is used to study the structure and stability of hybrid duplexes DNA•RNA and DNA•PNA in aqueous solution. Ribonucleic acid (RNA) is very similar to DNA, but differs in that RNA contains a ribose sugar ring while DNA contains deoxyribose. In addition all thymine bases are replaced by uracil in RNA. Peptide nucleic acid (PNA) is a DNA analogue that contains no sugar ring, and has an electrically neutral pseudopeptide backbone. DNA•RNA and DNA•PNA hybrid duplexes are biologically important molecules with potential therapeutic properties. Previous studies have shown that DNA•RNA and DNA•PNA duplexes are significantly stabilized when pyrimidine bases (thymine and cytosine) are attached to the DNA strand. In order to further investigate the stability and sequence-dependent structural effects, we performed molecular dynamics simulations using AMBER 9 on a series of DNA•RNA and DNA•PNA duplexes systems for which the purine base content of the DNA strand was systematically decreased from containing only purine to only pyrimidine bases. A comparison of the intramolecular entropy components of the backbones and bases of the various hybrids are analyzed in order to better understand the stability of DNA•RNA and DNA•PNA hybrid duplexes.

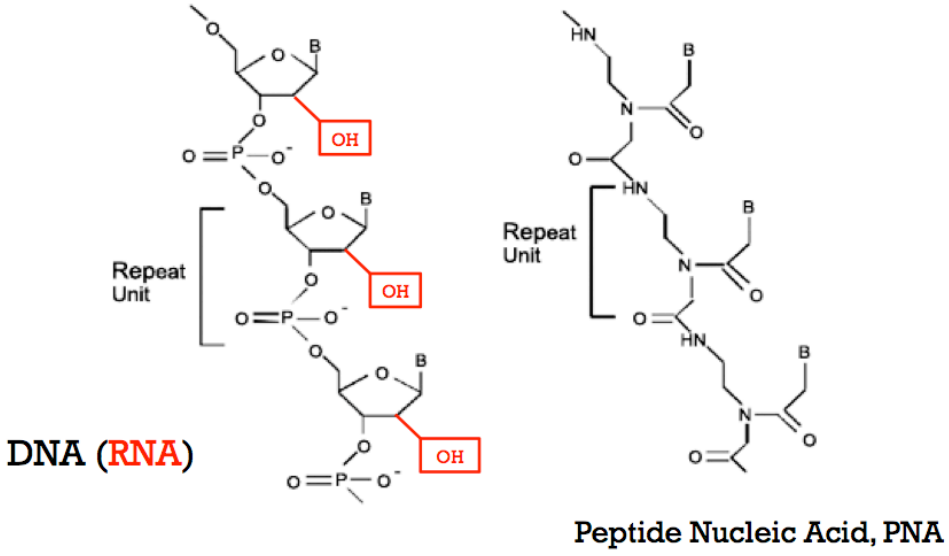

Figure 1: Comparison of backbone composition of DNA, RNA, and PNA.