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论文

DNA和RNA双链稳定性差异的理论研究

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摘要:

利用适用于分子间弱相互作用, 尤其是生物分子间的氢键相互作用的改进的半经验方法$RM1_{BH}$和达到线性标度的新的半经验算法以及SimuCal_SE方法, 与自主开发的量子化学程序包SimuPac 1.0, 对4组一系列DNA和RNA碱基的氢键结合能进行了计算. 这些计算包括单一碱基类型和混合碱基类型两大类情形, 最大的原子数达到1064个. 计算结果表明, 在碱基层数较少时, DNA和RNA氢键结合能差别不大; 在碱基层数较多时, RNA的氢键结合能明显高于DNA的氢键结合能; 嘌呤和嘧啶的排列方式对结合能略有影响, 但不影响上述趋势. 可见, 氢键对于RNA的稳定性差异起到重要的作用, 计算结果支持了实验的结论.

关键词: 半经验计算; RM1BH方法; SimuCal_SE方法; DNA 和RNA稳定性差异; 氢键结合能

Theoretical Study for DNA and RNA on Their Stability Difference

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Abstract:

The semi-empirical method $RM1_{BH}$, was employed to explore the reasons and nature of the intrinsic stability of the RNA and DNA duplexes. $RM1_{BH}$ is based on the convenient RM1 and modified to deal with the weak interactions between molecules, especially for the hydrogen bonding between biological systems, and embedded to our software module SimuCal_SE. And the calculations were processed using our software package SimuPac 1.0, with the linear scale algorithm to treat large molecular systems. The calculations in this study include 4 different sets of base pairs appeared in both DNA and RNA. By our calculations, the hydrogen bonding interaction energy of r(A\5U) is little bit larger than that of d(A\5T). When including more base pairs, the hydrogen bonding energies of RNA become much larger than DNA. Arrangements of purine and pyrimidine in RNA and DNA have contributions for the stabilities of both RNA and DNA. The calculation results in this study support and agree with the experimental results and conclutions.

Keywords: Semi-empirical calculation; RM1BH method; SimuCal_SE method; Stability difference of DNA and RNA; Hydrogen bonding energy

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