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抑制启动子的三链DNA的结构模建及稳定性研究

Stability and Molecular Modeling of Triplex DNA Inhibiting DNA Binding Protein Binding to the Core Promoter of Hepatitis B Virus

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英文关键词：triplex DNA　antigene strategy　homology modeling　core promoter　hepatitis B virus (HBV)

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中文摘要：

在IRIS Indigo2(SGI公司)工作站上，利用InsightⅡ/MSI软件包，以TAT三链DNA为模板，采用同源模建的方法，分别建立起两个含21nt的脱氧寡核苷酸CP1(G3TG2TGT2G5TG2TGT)和CP3(TGTG2TG5T2GTG2TG3)的三维结构.采用分子力学方法进行能量优化，将得到的能量最低结构作为分子的优势构象.研究结果显示，CP1的能量低于CP3的能量，即前者的结构较后者稳定.从而证明了CP1与乙肝病毒（HBV）的核心启动子（Cp）片段之间能稳定地形成三链DNA，并能特异性地抑制DNA结合蛋白与Cp片段的结合.这些结果表明，三链DNA的形成有可能抑制DNA的转录.

英文摘要：

Two three-dimensional structure models of the 21nt oligodeoxyribonucleotides, CP1 (G3TG-2TGT2G5TG2TGT) and CP3 (TGTG2TG5T2-GTG2TG3), were constructed by InsightII (MSI) software in IRIS Indigo2 (SGI) workstation using the crystal structure of TAT triplex formation as the template. The initial structures subsequently were minimized by molecular mechanics. The final structures were believed as the dominant conformation. The results showed that the energy of CP1 is lower than that of CP3, and the former is more stable than the latter. Moreover, the results further proved that the 21nt oligodeoxyribo-nucleotide CP1 stably combines with the core promoter (Cp) fragment of hepatitis B virus (HBV) to form a triplex DNA, and CP1 specifically inhibits a specific cellular factor (DNA binding protein) binding to Cp fragment. These results indicated that specific repression of gene transcription of HBV DNA might be possible by triplex-formation DNA.

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