

基于蛋白质-DNA复合物晶体结构的DNA结构动力学特性研究

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依据最新NDB数据库中蛋白质-DNA复合物晶体结构数据, 考虑DNA结构的序列依赖特性, 对10个二联体和36个约化的四联体计算了DNA动力学结构模型中的关键参数——力常数矩阵, 矩阵中的非对角项反映了结构参数间的关联。利用改进的DNA结构动力学模型, 可以方便地计算给定序列的结构动力学特性。

Study on DNA Dynamic Structural Feature Based on DNA-Protein Complex Crystal Data

Based on protein-DNA complex crystal structural data in up-to-date Nucleic Acid Database, taking into account the sequence-dependent feature of DNA, the key parameters in DNA dynamic structural model, force constant matrix, were calculated for 10 dimers and 36 tetramers. The non-diagonal elements represent the correlation between the structural parameters. One can calculate structural features, for example, curvature and flexibility, for given sequence using improved dynamic structural model.

关键词

蛋白质-DNA复合物(Protein-DNA complex); 晶体结构(Crystal structure); 力常数(Force constant); DNA; 动力学结构(Dynamic Structure)