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△,Λ-[Co(phen)2tpphz]^3+与B - DNA相互作用的分子 模拟

杨频,熊振海

山西大学分子科学研究所.太原(030006)

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摘要 针对国际上对金属配合物同DNA间作用机量的争议，采用分子模拟手段在MM2力场下，搭建并优化了手性金属配合物△,Λ-[Co(phen)2tpphz]^3+与B-DNA[d(GTCGATCGAC)2]的模型，继而对其相互作用进行了模拟，得出的结论是：对所采用的B-DNA片断，该金属配合物有明显的立体选择性△型配合物从小沟插入占明显优势，而且，总体来看，从AT区插入更易进行。

关键词 相互作用 金属络合物 二级结构 MM2力场 脱氧核糖核 钴络合物 探针 分子模拟

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Molecular modeling ofthe interaction between △,Λ -[Co(phen)2tpphz] ^3+ and B-DNA

Yang Pin,Xiong Zhenhai

Shanxi Univ., Inst of Mol Sci.Taiyuan(030006)

Abstract Molecular modeling methods have been applied to characterization of the interaction between a chiral metal complex [Co(phen)2tpphz]^3+ { where phen=1,10- phenanthroline, tpphz=tetrapyrido [3,2-a:2', 3'-c:3", 2"-h:2"', 3"'-j] phenazine} and an oligonucleotide (B- DNA fragment). The nature of two types of binding, a subject currently in controversy, was explored. Barton et al. proposed that there was enantioselective DNA binding by the octahedral complexes and intercalative access by these complexes from the major groove. Norden et al. suggested that both enantiomers bound extremely strongly to DNA from the minor groove without and noticeable enantioselectivity. Our results support and extend structural models of the minor groove based upon Norden's studies and Barton's enantioselectivity model.

Key words INTERACTIONS METAL COMPLEX SECONDARY STRUCTURE COBALT COMPLEX PROBES

DOI:

通讯作者