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论文

双金属存在下整合酶和抑制剂5CITEP的分子对接研究

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摘要:

在HIV-1整合酶(IN)和5CITEP复合物晶体结构的基础上, 用分子对接程序(Affinity)将含有单Mg^{2+}和双Mg^{2+} 的HIV-1 IN核心区与抑制剂5CITEP进行对接, 获得了能形成复合物结构的理论模型. 通过配体与受体之间的相互作用能和结构分析给出此种抑制剂的结合模式, 并与晶体结构进行比较， 揭示出引入的第二个Mg^{2+}原子在整合过程中所起的重要作用. 前后相互作用能的变化趋势很明显, 配体和受体的作用模式比单Mg^{2+}体系更加清晰. 由单Mg^{2+}体系的4种作用方式改变到双Mg^{2+}体系的两种作用方式, 相互作用能提高了将近40 kJ/mol. 为基于整合酶结构的药物设计提供了参考信息.

关键词： HIV-1整合酶(IN)； 分子对接； 双金属

Molecular Docking Study of HIV-1 IN/Inhibitor in the Presence of Double Metal Conditions

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Abstract:

Based on a crystallographically resolved HIV-1 IN/inhibitor complex, the complex structures of the 5CITEP inhibitor with the crystal structure of HIV-1 IN which contains a single metal and double metal were obtained and investigated through ligand-receptor docking studies by means of a molecular docking program called Affinity. The binding pattern predicted by the affinity module reveals that the second metal is of importance during integration, provides a further refinement of the IN/inhibitor binding interaction as a basis for new structure-based design efforts. There exists an obvious difference between the two systems about the interaction energy, the value of the latter is lower than that of the former by about 40 kJ/mol. The patterns of interaction between the ligand and the receptor reduces the two probabilities from the previous four ones.

Keywords: HIV-1 IN Molecular docking Double metals

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