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## 论文

### 乙型肝炎病毒表面抗原三维结构的同源模建及功能预测

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#### 摘要:

结合生物信息学方法及分子模拟手段, 通过同源模建方法构建了乙型肝炎病毒表面抗原(HBsAg)Pres12的三维空间结构, 并结合生物实验在分子水平上探讨了乙型肝炎病毒表面抗原Pres12作为抗乙型肝炎病毒重要靶标的机理. 研究表明, HBsAg三维空间结构是由构型性的Pres1和线性的Pres2组成, 此结构由疏水氨基酸形成3个 $\alpha$ -螺旋结构及Loop结构域, 并且N端由Pres1中残基构成了一个开裂, 形成了HBsAg可能的活性部位. 静电势分析结果证实, N端可能的活性部位具有较大的静电势分布, 因而具有与受体细胞蛋白相互作用的能力, 这为HBV病毒抑制剂药物分子的设计提供了有益帮助.

关键词: 乙型肝炎; 表面抗原; 同源模建; 分子对接; 静电势

### Homology Model and Functional Prediction of the Three Dimensional Structure of HBsAg of Hepatitis Virus

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#### Abstract:

When hepatitis B virus(HBV) conduct the planting process into normal liver cell, hepatitis B virus surface antigen(HBsAg) plays an important role during this process, but its crystal structure information has not been reported in the Protein Data Bank. In order to make further research about the structure and function of HBsAg, we constructed the three dimensional structure of HBsAg Pres12 using biology information homology model methods, and explored the mechanism as an important antiviral target at the molecular level by molecular simulation method. The results showed that the three dimensional structure of HBsAg consist the conformational Pres1 and the linear Pres2, three  $\alpha$ -helixes and some loop region consist the whole structure, at the same time, some amino residues in the N-terminal of Pres1 make a cleft which forms the potential active site domain. The electrostatic analysis confirmed that, the N-terminal potential active site possess bigger electrostatic distribution and may have the ability to interact with recipient cell protein, this study will provide useful information for the design of anti-HBV drug molecules.

Keywords: Hepatitis B; Surface antigen; Homology modeling; Molecular docking; Electro-static potential

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