高等学校化学学报 2007 28 (5): 971—973 ISSN: 0251-0790 CN: 22-1131/O6

研究简报

Thermus thermophilus 木糖异构酶与木糖醇的分子对接及模型分析

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收稿日期 2006-6-5 修回日期 网络版发布日期 2007-4-23 接受日期

摘要 在1BXB结构基础上, 通过分子对接方法构建木糖异构酶与抑制剂木糖醇的复合物模型, 为合理设计解除木糖醇对木糖异构酶的抑制及进一步揭示木糖醇对该酶抑制机理提供参考.

关键词 嗜热栖热菌 木糖异构酶 木糖醇 分子对接

分类号 O641 Q71

DOI:

Molecular Docking of Xylitol and Xylose Isomerase from *Thermus thermophilus* and Model Analysis

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Received 2006-6-5 Revised Online 2007-4-23 Accepted

Abstract Xylose isomerase from *Thermus thermophilus* is widely used in the production of high-fructose corn syrup and the construction of xylose *via* recombinant strains. In this paper, the positions of Mg ions and xylitol in 1BXB were established by structure analysis, molecular docking and computing. The Complex of 1BXB with xylitol was modeled and analyzed. Comparing the structure of 1BXB complex with 1S5N, it was found that the overall structure of them showed a high similarity. The residues around xylitol were highly conserved in xylose isomerase, and the orientation and positions of xylitol were very similar in both structures. The coordination bonds formed between Mg1 and O2 or O4 of xylitol stabilized the conformation of xylitol at the active site of 1BXB.

Key words *Thermus thermophilus*; Xylose isomerase; Xylitol; Molecular docking

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