

RESEARCH ARTICLE

Chiral recognition mechanism of cellobiohydrolase Cel7A for ligands based on the β -blocker propranolol: The effect of explicit water molecules on binding and selectivities

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Abstract

Proteins are useful chiral selectors. In order to understand the recognition mechanism and chiral discrimination, the binding of the (*R*)- and (*S*)-enantiomers of a series of designed amino alcohol inhibitors based on propranolol to cellobiohydrolase Cel7A (*Trichoderma reesei*) has been studied more closely. X-ray crystal structures were determined of the protein complex with the (*R*)- and (*S*)-enantiomers of the strongest binding propranolol analogue. The combination of the structural data, thermodynamic data from capillary electrophoresis and microcalorimetry experiments and computational modelling give a clearer insight into the origin of the enantioselectivity and its opposite thermodynamic signature. The new crystal structures were used in computational molecular flexible dockings of the propranolol analogues using the program Glide. The results indicated that several water molecules in the active site were essential for the docking of the (*R*)-enantiomers but not for the (*S*)-enantiomers. The results are discussed in relation to the enantiomeric discrimination of the enzyme. Both dissociation constants (K_d values) and thermodynamical data are included to show the effects of the structural modifications in the ligand on enthalpy and entropy in relation to the enantioselectivity.

KEYWORDS

Cel7A, computational chemistry, enantioselectivity, inhibitor binding, propranolol, thermodynamics

INTRODUCTION

Access to enantiomerically pure material is of great importance in many scientific areas, particularly in biology and medicine. This can be accomplished either through asymmetric synthesis or by separation of the enantiomers from the racemic mixture. Proteins have been

successfully used as chiral selectors in liquid chromatographic and capillary electrophoretic techniques to determine the enantiomeric composition of various drugs.¹ However, in most cases, it is difficult to foresee affinity and selectivity in the interplay between the enantiomers and the protein (selector), as well as which kind of interactions that are involved. This requires determination of the influence of different functionalities of the ligands, which amino acid residues of the protein are involved in the chiral discrimination and how flexible the

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Cellobiohydrolase I As A Chiral Selector

IM Harris



Cellobiohydrolase I As A Chiral Selector:

The book delves into Cellobiohydrolase I As A Chiral Selector. Cellobiohydrolase I As A Chiral Selector is a vital topic that needs to be grasped by everyone, from students and scholars to the general public. The book will furnish comprehensive and in-depth insights into Cellobiohydrolase I As A Chiral Selector, encompassing both the fundamentals and more intricate discussions.

1. The book is structured into several chapters, namely:
 - Chapter 1: Introduction to Cellobiohydrolase I As A Chiral Selector
 - Chapter 2: Essential Elements of Cellobiohydrolase I As A Chiral Selector
 - Chapter 3: Cellobiohydrolase I As A Chiral Selector in Everyday Life
 - Chapter 4: Cellobiohydrolase I As A Chiral Selector in Specific Contexts
 - Chapter 5: Conclusion
 2. In chapter 1, the author will provide an overview of Cellobiohydrolase I As A Chiral Selector. This chapter will explore what Cellobiohydrolase I As A Chiral Selector is, why Cellobiohydrolase I As A Chiral Selector is vital, and how to effectively learn about Cellobiohydrolase I As A Chiral Selector.
 3. In chapter 2, this book will delve into the foundational concepts of Cellobiohydrolase I As A Chiral Selector. The second chapter will elucidate the essential principles that need to be understood to grasp Cellobiohydrolase I As A Chiral Selector in its entirety.
 4. In chapter 3, this book will examine the practical applications of Cellobiohydrolase I As A Chiral Selector in daily life. This chapter will showcase real-world examples of how Cellobiohydrolase I As A Chiral Selector can be effectively utilized in everyday scenarios.
 5. In chapter 4, the author will scrutinize the relevance of Cellobiohydrolase I As A Chiral Selector in specific contexts. This chapter will explore how Cellobiohydrolase I As A Chiral Selector is applied in specialized fields, such as education, business, and technology.
 6. In chapter 5, this book will draw a conclusion about Cellobiohydrolase I As A Chiral Selector. The final chapter will summarize the key points that have been discussed throughout the book.
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