

## RESEARCH ARTICLE

# Chiral recognition mechanism of cellobiohydrolase Cel7A for ligands based on the $\beta$ -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.<sup>1</sup> 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

<sup>†</sup>Deceased author.

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# Cellbiohydrolase I As A Chiral Selector

**Peipei Pang**



## **Cellobiohydrolase I As A Chiral Selector:**

## Whispering the Secrets of Language: An Mental Journey through **Cellobiohydrolase I As A Chiral Selector**

In a digitally-driven world wherever screens reign supreme and quick transmission drowns out the subtleties of language, the profound secrets and emotional nuances hidden within phrases usually move unheard. However, situated within the pages of **Cellobiohydrolase I As A Chiral Selector** a charming literary value sporting with organic thoughts, lies an exceptional quest waiting to be undertaken. Written by a talented wordsmith, that charming opus invites viewers on an introspective journey, gently unraveling the veiled truths and profound influence resonating within ab muscles cloth of each word. Within the psychological depths of the emotional evaluation, we will embark upon a genuine exploration of the book is core themes, dissect its fascinating writing model, and fail to the effective resonance it evokes strong within the recesses of readers hearts.

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