

# **The influence of metal ions on the substrate binding pocket of human alcohol dehydrogenase B2B2 by molecular modeling**

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## **Abstract**

Based on theoretical molecular modeling performed in this study, both structural and catalytic zinc ions, Zns and Zna, respectively, were shown to influence the structural integrity of the substrate binding pocket of human alcohol dehydrogenase b2b2 in the middle and outer regions. The replacement of both Zns and Zna with different metal ions restricts the access of bulky substrates to the bottom of the active site by narrowing the bottleneck formed between L116 and V294, whereas it does not affect substrate binding affinity since the accessible surface area of the substrate binding pocket remains more than 80% of the wild-type.