

# Docking investigation and binding interaction of camphor with alanine aminotransferase (ALT)

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## ABSTRACT

Camphor as a herbal medicine has many various physiological effects. It is used for different purposes such as stimulation of circulatory and respiratory systems and also affects skin, reproductive system, liver and kidney. The effect of camphor on Alanine aminotransferase (ALT), Aspartate amino-transferase (AST), Alkaline phosphatase (ALP) and Creatine Kinase (CK) blood enzymes has been conducted. ALT and AST are the most important enzymes in group of trans-amines. They transfer the amin group and then catalyze the process of transforming  $\alpha$ -keto acids into amino acids. ALT is a specific factor in liver for defining the liver damage. It is only increased in the liver of patients, but AST acts not only as a factor in liver damage but also is increased in heart damages.

In this work we interested in finding any interactions between camphor and ALT enzyme. Molecular docking technique is an attractive scaffold to understand the ligand–protein interactions which can substantiate the experimental results. Camphor is capable of existing in both the keto form and the enol form. Usually, the keto form is more stable than the enol form. The crystal structure of ALT (PDB entry 3IHJ) is obtained from the Protein Data Bank (<http://www.rcsb.org/pdb>). The binding interactions of camphor with ALT were simulated by molecular docking using Auto Dock 4.0. The molecular docking results and the dominating configuration of the binding complex of camphor with ALT, which was the lowest binding free energy, were obtained.

**Key words:** Camphor, Alanine aminotransferase (ALT), Molecular docking