

# MOLECULAR MODELING AND DOCKING STUDY OF ACETYLCHOLINESTERASE FROM *Camelus dromedarius*

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## ABSTRACT

The acetylcholinesterase (AChE) is the essential enzyme to hydrolyse the neurotransmitter acetylcholine (ACh) in central neural system (CNS). In our study, homology modeling method was used to model the 3D structure of AChE from *Camelus dromedarius*. The obtained model was evaluated and verified. Analysis of its structure and electrostatic potential showed that the AChE from *Camelus dromedarius* consisted of 14 alpha-helices and 13 beta-sheets forming a gorge with a negative value of electrostatic potential. Structure alignment of AChE from different animal species showed their remarkable similarity. The results of molecular docking performed by Autodock 4.0 showed that ACh binds with the acetylcholinesterase at the gorge with the active site which contained S203, E334 and H447 residues similar to the catalytic triad of most serine proteases.

**Keywords:** Acetylcholinesterase, *Camelus dromedarius*, docking, molecular modeling