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Ureido histamine as activator of carbonic anhydrase (I) enzyme: A DFT investigation

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ABSTRACT

Activation mechanism of human carbonic anhydrase (hCA) isoform I, with ureido histamine has been investigated by using quantum mechanical calculations. The B3LYP/6-31G method have been employed to calculate the details of electronic structure and electronic energy of active and inactive forms of carbonic anhydrase enzyme active center, isoform I (CA). ureido histamine activator of this enzyme and complex between this activator and active center of carbonic anhdrase have been investigated. The calculated results indicate that protonatable moiety of ureido histidine molecule participate in proton transfer from zinc-bound water molecule and lead to formation of the catalytically active species of CA enzyme, hydroxide coordinated to the zinc ion.*

Keywords: DFT calculation, Carbonic anhydrase, Ureido histamine, Activator

1. INTRODUCTION

Proton transport is an important event in many biological processes that are influenced by environmental electrostatic charges [1-3]. One class of biological enzymes that facilitate the proton transport is carbonic anhydrase (CA) family. The carbonic anhydrase (CA, EC 4.2.1.1) belong to a family of zinc metalloenzymes that catalyze the reversible conversion of carbon dioxide to bicarbonate [4], Figure 1.

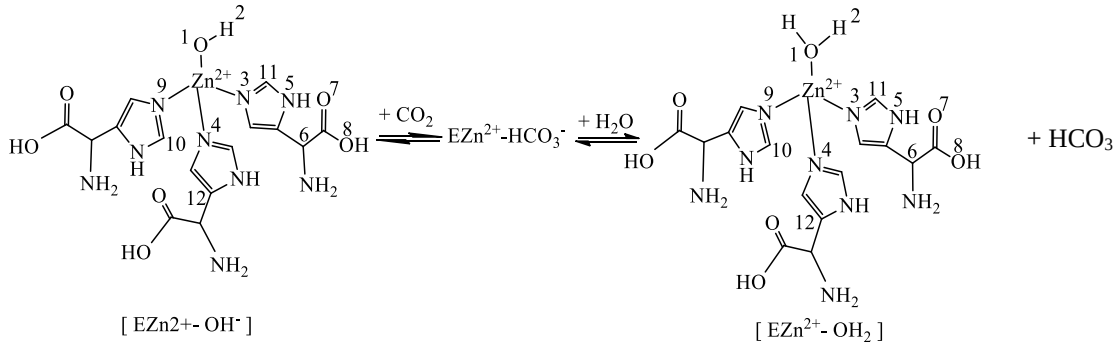

Fig .1. *Schematic representation of the catalytic mechanism for the CA catalyzed CO_2 hydration.*