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Interaction energy and electronic structural details of complexation between azide as an anionic inhibitor and active site of α-CA enzyme: DFT study

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ABSTRACT

*Density functional theory (DFT) using B3LYP functional and split-valance 6-311G** basis set have been used to optimized the structures of azide inhibitor and complex between this inhibitor with active site of α-carbonic anhydrase (CA) enzyme. According to predicted results the zinc cation in the active site of the CA enzyme prefers tetrahedral geometry. While the azide anion is coordinated to the zinc, the geometry could be change to trigonal bipyramidal or the tetrahedral geometry. Also the azide anion belongs the second group of inhibitors of α-carbonic anhydrase which possess pharmacological applications.*

Keywords: DFT calculation, Carbonic anhydrase, Azide, Inhibitor, Anticancer

1. INTRODUCTION

Carbonic anhydrases belong to biological metalloenzymes that facilitate the proton transport and present in all three domains of life (Eucarya, Bacteria and Archaea) which are encoded by five distinct, evolutionarily gene classes: α-CAs, β-CAs, γ-CAs, δ-CAs and ζ-CAs [1-5]. The α-, β-, and δ-CAs use zinc ion (Zn(II)) at their active site, Fig. 1 [6-9]. the γ-CAs are mostly Fe(II) and Co(II) enzymes but they are active also when Zn^{2+} ions bond, whereas the ζ-CAs use Cd^{2+} or Zn^{2+} to perform the physiologic reaction catalysis [6-12].

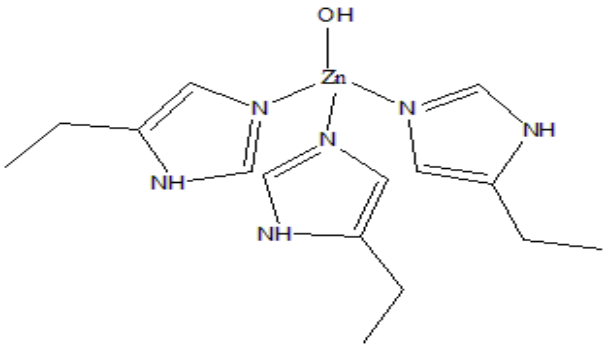

Fig .1. *Presentation of zinc enzyme carbonic anhydrase active center(CA)*