عنوان مقاله:

The inhibition of α-carbonic anhydrase (CA) enzyme by cyanate ion with five-fold ligand: A DFT study

محل انتشار:

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خلاصه مقاله:

Density functional theory (DFT) using B3LYP functional and split-valance 6-311G** basis set have been employed tooptimized the geometry ofcyanate ion (OCN^-)inhibitor and complex between this inhibitor with active site of α-carbonic anhydrase (CA) enzyme. The results show that the zinc cation in the active site of the CA enzyme prefers tetrahedral geometry. While the cyanate anion is coordinated to the zinc, the geometry could be change to trigonal bipyramidal or the tetrahedral geometry [1,2],(Figure 1).It is noteworthy that among the anions studied as inhibitors, including: $N3^-$, SCN^-, HS^-, $HSO3^-$, CN , cyanateion performs the best inhibitor.Also the cyanateanion belongs the second group of inhibitors of α-carbonic anhydrase which possess pharmacological applications.

کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا: