عنوان مقاله:

QM Study on the Mechanism of Carbonic Anhydrase XII Inhibition with Glycosyl Coumarin as Non-Zinc Mediated Inhibitors

محل انتشار:

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خلاصه مقاله:

Metalloenzyme carbonic anhydrases (CAs, EC 4.2.1.1) present in prokaryotes andeukaryotes which is encoded by three distinct gen families: (i) α-CA, (ii) β-CA and (iii) γ-CAs.In recent years a novel group of inhibitors of CA that belong to the new chemotype moleculesincluding coumarins and their derivatives have been reported [1, 2]. In this research, inhibitionmechanism of zinc enzyme carbonic anhydrase XII (CA XII) by a novel class of suicideinhibitors, glycosyl coumarin, has been modeled using of density functional theory DFT at theB3LYP level using 6-31+G* basis set to study the electronic structures and thermocemicalaspects of this mechanism. In the first step of this research the most stable conformer of 7-substituted sugar coumarin, melibiose coumarin as more effective and coumarin as the lesseffective inhibitor of CA XII respectively has been search and interact with CA XII active site.The results of calculations indicate that mentioned inhibitor do not directly interact with themetal ion from the CA active center. Moreover, the calculated thermodynamic function valuesindicate the presence of sugar moiety in the coumarin molecule was associated with moreeffective inhibition [3, 4]. In addition the good agreements between the calculated .results withexperimental data indicate a reliable agreement of method of calculations

کلمات کلیدی:

Carbonic Anhydrase, Glycosyl Coumarin, Inhibition Mechanism, QM Calculation