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عنوان مقاله:

Quantum mechanical study on the inhibition mechanism of carbonic anhydrase biocatalyst in the presence of coumarin inhibitors

محل انتشار:

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خلاصه مقاله:

In the present study the inhibition mechanism of zinc enzyme carbonic anhydrase XII (CAXII) by new class of suicide inhibitorsm coumarin derivatives, has been modeled using ofdensity functional theory (DFT) to study the geometrical parameters and thermocemicalaspects of this mechanism in the solution phase. The results of our calculations indicatethat studied inhibitors do not directly interact with the metal ion from the CA active center.In addition the good agreements between our calculated results with experimental dataindicate a reliable agreement of method of .calculations

کلمات کلیدی:

Carbonic anhydrase, Biocatalyst, Coumarin, DFT calculations

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