

عنوان مقاله:

Cyclodextrin solubilization of dorzolamide as an effective inhibitor of CA enzyme: QM study

محل انتشار:

ششمین کنگره ملی تحقیقات راهبردی در شیمی و مهندسی شیمی با تاکید بر فناوری های بومی ایران (سال: 1398)

تعداد صفحات اصل مقاله: 3

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خلاصه مقاله:

In this work, the complex formed between γ -cyclodextrin (γ -CD) and dorzolamide (one of the most effective inhibitor of carbonic anhydrase enzyme) was investigated by using quantum mechanical calculations. The complex between dorzolamide and γ -cyclodextrin from different directions were fully optimized by using B3LYP/6-31G method. According to our calculated results, dorzolamide forms a complex with γ -CD with the stoichiometry of 1:1. Negative stability energy indicate that the inclusion of dorzolamide with γ -CD cavity is spontaneously and refer to formation of hydrogen bonds between host and guest molecules. More detailed understanding of the inclusion mechanism of dorzolamide would allow us to design more specific cyclodextrin derivatives with better affinity and functionality towards this kind of inhibitors.

کلمات کلیدی:

γ -cyclodextrin, dorzolamide, Inclusion complex, CA enzyme, QM calculations

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