

## عنوان مقاله:

Theoretical study on the effect of glycoside group on Antioxidant ability of Chrysin

## محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

تعداد صفحات اصل مقاله: 3

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## خلاصه مقاله:

Chrysin (1), Chrysin-6-C-fucopyranoside (2), and Chrysin-3-malonyl-6-C-fucopyranoside (3), bioflavonoids, were selected to theoretical study on the effect of glycoside group on the BDE (Bond Dissociation Energy) values and  $\Delta E$  (ELUMO – EHOMO). The calculation of the theoretical bond dissociation enthalpy (BDE) and energy gap ( $\Delta E$ ) were carried out in B3LYP/6-311++G\*\* level. The BDE and  $\Delta E$  values for these three compounds were calculated. Our results indicated that antioxidant ability of flavonoid did not change in the presence of glycoside group

## کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/552601>

