

## عنوان مقاله:

Dipolar Cycloaddition Reactions on Medicine Dimethisterone: A Computational Insight-1,3

## محل انتشار:

بیست و ششمین سمینار شیمی آلی ایران (سال: 1397)

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## خلاصه مقاله:

The different types of 1,3-dipolar cycloaddition (1,3-DC) reactions have been widely used in various fields. Based on the recent researches, stereochemistry of these reactions is spotlight[1]. In this study, the theoretical aspects of the electrostatic attraction effect on the regioselectivity of the 1,3-DC reactions to dimethisterone was assessed which it is a progestin medication[2] as a dipolarophile with nitrile imine (a), nitrile oxide (b) and azide (d) as 1,3-dipoles. Cycloaddition of dimethisterone to each of a-d can lead to regioselective five-membered heteroaromatic rings, the 4- and/or 5-substituted, due to secondary effect between the hetero atom of 1,3-dipoles and the hydroxy group in dimethisterone. These heteroaromatic rings were widely used as an important role in various biochemical processes [3]. In this study, the (1,3-DC) reaction of dimethisterone with a-d were utilized to produce the five-membered aromatic heterocyclic rings, i.e. pyrazole, isoxazole and triazole derivatives. Data were calculated and obtained by DFT-B3LYP/6-31G\* method.

## کلمات کلیدی:

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