



ZABOL UNIVERSITY

Faculty of Sciences

Department of Chemistry

Subject:

Computational study on the effect of π - π stacking on the intramolecular hydrogen bonding interactions in some flavonoid derivatives and their role in the anticancer activity of these compounds

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Abstract

Studies have shown that compounds derived from plants are particularly important in the treatment of various diseases. One group of these compounds are flavonoids, which are one of the largest groups of polyphenols found in plants and include a wide range of medicinal activities, including anticancer. In this work, the effect of pi-pi stacking interactions on intramolecular hydrogen bonds in some flavonoid derivatives is investigated. Also, the importance of these interactions in the anticancer activity of these compounds is investigated by molecular docking calculations. The results obtained from this research confirmed that there is almost an inverse relationship between the strength of pi-pi stacking interactions and intramolecular hydrogen bonds in flavonoids and it can be said that the increase in pi-pi stacking interactions decreases the tendency of flavonoids to participate in the intramolecular hydrogen bonds and increases intermolecular ones.