

Accepted Manuscript

Theoretical prediction of chloroform, ethanol, water and DMSO effects on electronic characteristics of Capecitabine different conformers as an anticancer chemotherapy drug

Mehdi Yoosefian, Adeleh Mola, Hossein Hajiabadi, Rouhollah Amiri Delouei



PII: S0167-7322(17)35636-2
DOI: doi:[10.1016/j.molliq.2018.04.115](https://doi.org/10.1016/j.molliq.2018.04.115)
Reference: MOLLIQ 9018
To appear in: *Journal of Molecular Liquids*
Received date: 22 November 2017
Revised date: 2 March 2018
Accepted date: 23 April 2018

Please cite this article as: Mehdi Yoosefian, Adeleh Mola, Hossein Hajiabadi, Rouhollah Amiri Delouei , Theoretical prediction of chloroform, ethanol, water and DMSO effects on electronic characteristics of Capecitabine different conformers as an anticancer chemotherapy drug. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:[10.1016/j.molliq.2018.04.115](https://doi.org/10.1016/j.molliq.2018.04.115)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Theoretical prediction of chloroform, ethanol, water and DMSO effects on electronic characteristics of Capecitabine different conformers as an anticancer chemotherapy drug

Mehdi Yoosefian^{*a}, Adeleh Mola^b, Hossein Hajiabadi^c, Rouhollah Amiri Delouei^d

^a Department of Nanotechnology, Graduate University of Advanced Technology, Kerman, Iran

^b Department of Medical Chemistry, Faculty of Pharmacy, Kerman University of Medical Sciences, Kerman, Iran

^c Department of Chemistry, Faculty of Science, University of Sistan and Baluchestan (USB), P.O.Box 98135-674, Zahedan, Iran

^d Department of Physics, Gonabad Branch, Islamic Azad University, Gonabad, Iran

***Corresponding author.**

E-mail address: myoosefian7@gmail.com

Abstract

In this study, the solvent effects on the structures and strength of intramolecular hydrogen bonds (HBs) of capecitabine conformers were investigated using density functional theory. The achieved results show the hydrogen bonds strongly affect the stability order of conformers so that IHB strength among the solvents is increased as: chloroform > ethanol > water > DMSO. Also, A₁ and A₃ conformers are stabilized more than other conformers in gas phase and solution phase respectively. This stability with increase of dielectric constant is lessened. The natural bond orbital and the Quantum Theory of “Atoms in Molecules” (QTAIM) of Bader were also applied to achieve more details about the nature of intermolecular and HB interactions. Finally, electronic descriptors such as energy gap, hardness, softness and chemical potential were investigated.

Keywords: Capecitabine; Solvent effect; density functional theory; breast cancer; chemotherapy drug.

1. Introduction

In spite of low energy (in kilocalorie per mole) of hydrogen bonds (HBs), the structure and properties of many molecules participating in this interaction are strongly influenced by them [1-

Download English Version:

<https://daneshyari.com/en/article/7842043>

Download Persian Version:

<https://daneshyari.com/article/7842043>

[Daneshyari.com](https://daneshyari.com)