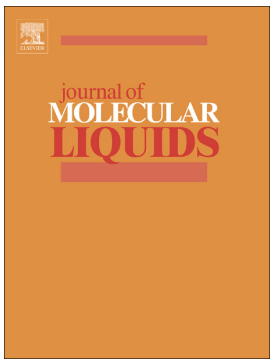

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Mehdi Yoosefian, Adeleh Mola, Hossein Hajiabadi, Rouhollah Amiri Delouei

PII: S0167-7322(17)35636-2
DOI: doi: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

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, A_1 and A_3 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-