Goncagul Serdaroglu, Mod Chem Appl 2018, Volume: 06
DOI: 10.4172/2329-6798-C1-008

A computational approach on the structural, electronic, and spectroscopic properties of the aromatic substituted indole alkaloids

Goncagul Serdaroglu

Sivas Cumhuriyet University, Turkey

The indole alkaloids and heterocyclic aromatic compounds have a vital role in research fields such as chemistry, pharmacology and biology etc., because of the structural properties of them; they have acted (agonist or antagonist) on variety of receptor sites on CNS (central nervous system). Recently, the computational tools are getting commonly used to explain the reactivity behavior of a specific molecular system. All quantum chemical calculations by using the DFT method with G09W package have been conducted at three basis sets and ten solvents to look for the basis set and solvent effect on the chemical reactivity behavior of each studied aromatic heterocyclic compounds. The solvation phase simulations have been performed by PCM (Polarized Continuum Model). The aromatic substituent group effects on the intra-molecular charge transfer of the basic structural unit have been evaluated by NBO analysis. The functional group vibrational modes verifying by GaussView 4.1program are a good agreement with the literature data. The HOMO, LUMO and MEP diagrams have used to predict the nucleophilic and electrophilic attack sites of each studied compounds. The physicochemical parameters and quantum chemical parameters of aromatic substituted compounds have been calculated to compare with the basic structural unit the chemical reactivity behavior of all compounds, too. All calculations have been conducted at Tubitak Ulakbim, High Performance and Grid Computing Center. The author thanks to Scientific Research Projects Department of Cumhuriyet University (Project No: CUBAP: EĞT-066).

Biography

Goncagul Serdaroglu has completed her PhD from Cumhuriyet University, in 2008 and Post-doctoral studies from Auburn University, in 2014. Her research interests are on the electronic structure methods and their applications to the medicinal and pharmacologically important molecules. Recently, she has also focused on spectroscopic investigation of organic molecules by using computational tools.

Goncagul.serdaroglu@gmail.com

Notes: