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The structural, electronic, and spectroscopic properties of the potential neuroactive alkaloids: a computational study

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Neuroactive alkaloids have a variety of the pharmaceutical importance because of acting on receptor sites on central nervous system (CNS). The geometric structure optimizations in the gas phase and frequency calculations of each alkaloid have been employed by G09 package. First, the optimized geometries obtained from gas phase calculations of each alkaloid have been used re-optimized in the five different solvents by using the Polarized Continuum Model (PCM) to look for the solvent effect on physicochemical and quantum chemical parameters. Also, the optimized geometry of each compound has been verified by no imaginary frequency in all solvents as well as the gas phase. The important intra-molecular interactions have been evaluated by NBO analysis. The vibrational modes of each compound have been verified by GaussView 4.1 software. The quantum chemical descriptors have been used to predict the chemical stability and reactivity behavior of each compound. Moreover, the MEP diagrams and HOMO, LUMO amplitudes have been illustrated to show the nucleophilic and electrophilic attack site of each compound. All calculations have been conducted at Tubitak Ulakbim, High Performance and Grid Computing Center.

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.

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