

A pair of carbazate derivatives as novel Schiff base ligands: DFT and POM theory supported spectroscopic and biological evaluation

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ABSTRACT

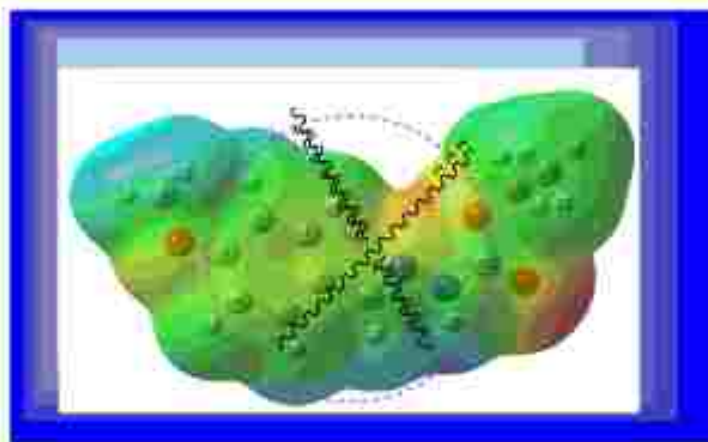
Schiff bases are mentioned as strongly important molecular scaffolds of industrial and medicinal purposes. Due to wide range applications of carbazate derivatives herein synthesis and characterization of a new Schiff base ligand, (E)-ethyl 2-(4-methoxybenzylidene)hydrazisecarboxylate and 4-(nitrobenzaldehyde)ethylcarbazate are reported. The compound was characterized on the basis of experimental and density functional theory calculations (using the B3LYP and 6-31 G(d,p) formalism combination). Among characterization techniques elemental analysis, FT-IR, UV-Vis and NMR spectroscopic evaluations were mainly employed to carry out the formulation of the compound. In addition to computational validation of characterization other significant molecular parameters were also evaluated including geometry optimization, frontier molecular orbital analysis (FMO) and Columbic interaction of different constituent atoms of the title compound. A good agreement has been found between DFT and experimental outcomes confined to prove the structure of the compound. Moreover, molecular docking and antimicrobial studies have proven the Schiff base as an effective bioactive compound.

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Introduction

Schiff bases recognized as high biological implications that have an intensive interest in bioinorganic chemistry and medicinal chemistry (Nagpal & Singh, 2004). Schiff bases derived carbazate derivatives are interesting molecules of diverse applications (Ali et al., 1977; Chen et al., 2015; Hamid et al., 2009; Maurya et al., 1992, 2002; Maurya, 2006; Singh & Tripathi,

1988; Tarafder et al., 2001, 2002). This class of compounds comprises of potential pharmacophores displaying wide variety of bonding modes of stereochemistry. A wide variety of stable metal complexes can be formed from dithiocarbazate ligands by introducing different organic substituents to dithiocarbazate ligand (Casas et al., 2015). 5-methyldithiocarbazate (SMOTC) Schiff bases has been reported to be effective against MDA MB-

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