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ORIGINAL PAPER

Synthesis and evaluation of molecular structure from torsional scans, study of molecular characteristics using spectroscopic and DFT methods of some thiosemicarbazones, and investigation of their anticancer activity

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Abstract
Synthesis of 2-((2-aminopyridin-3-yl) methylene) hydrazinecarbothioamide (APHT) was attempted. Elemental analysis and NMR spectra were used to ascertain its formation. Torsional potential energy scans for all five of its rotating bonds were made to get approximate dihedral angles. UV–Vis spectra were measured for APHT and 2-((2-aminopyridin-3-yl) methylene)-*N*-methylhydrazinecarbothioamide (APMHT). Their anticancer activity was determined experimentally, for human carcinoma cell lines pertaining to liver, colorectal, and lung. For both APHT and APMHT, frontier molecular orbital parameters, NLO behaviour, and NBO characteristics were determined using DFT/B3LYP/6-311++G(d,p) level of theory. TD-DFT was used to compute absorption maxima (λ_{max}) of electronic transitions for both molecules in DMSO-d_6 solvent. Frontier molecular orbitals were used to understand origin of UV–Vis spectra and chemical reactivity of the two molecules. Good agreement was found between measured and computed structure parameters. This is also true of experimental and theoretical UV–Vis spectra. The computations demonstrated that both the molecules were good for NLO applications, which was substantiated by NBO analysis. Existence of bifurcated intramolecular hydrogen bond was predicted for both APHT and APMHT.

Keywords Hydrazinecarbothioamides · Torsional potentials · Barrier heights · Vibrational spectra · DFT · Anticancer activity

Introduction

Heterocyclic thiosemicarbazones are known for their therapeutic value (Blanz et al. 1970) and biological activity (El-Sharief and Moussa 2009), such as antitumour (Cao et al. 2005), anticonvulsant (Jatav et al. 2008), antifungal (Tiwari et al. 2007), anti-inflammatory (Giri et al. 2009), antibacterial (Yousef et al. 2013), antituberculosis (Mohamed et al. 2004), antiviral (Padmapriya et al. 2016), analgesic (Van Zyl 2001) and HIV-TB coinfection effects (Banerjee et al. 2011). A brief account of some of these biological activities is worth reporting. For instance, a study of formyl thiosemicarbazones having different heterocyclic systems confirmed that their anticancer activity arose from the side chain adjacent to the heterocyclic nitrogen atom and conjugated NNS tridentate ligand system of thiosemicarbazone (Blanz et al. 1970). It was found that the antifungal activity exhibited by metal complexes of thiosemicarbazones was decided by the substituent group at N(1) and N(4) positions of the thiosemicarbazone (West et al. 1993). This prompted intense research activity involving 2-formylpyridine, 2-benzopyridine and 2-acetylpyridine N(4)-substituted thiosemicarbazones (West et al. 1994, 1995; Liberta and West 1992). The utility of the thiosemicarbazones as antimicrobial inhibitors

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