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Research Article

Spectroscopic Investigations, DFT Calculations, and Molecular Docking Studies of the Anticonvulsant (2*E*)-2-[3-(1*H*-Imidazol-1-yl)-1-phenylpropylidene]-*N*-(4-methylphenyl)hydrazinecarboxamide

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Drug discovery for the management of neurological disorders is a challenging arena in medicinal chemistry. Vibrational spectral studies of (2*E*)-2-[3-(1*H*-imidazol-1-yl)-1-phenylpropylidene]-*N*-(4-methylphenyl)hydrazinecarboxamide ((2*E*)-IPPMP) have been recorded and analyzed to identify the functional groups and intermolecular/intramolecular interactions of the title molecule. The blue shift of the C-H stretching wavenumber reveals the presence of improper C-H$\cdots$O hydrogen bonding. The equilibrium geometry, harmonic vibrational wavenumbers, Frontier orbital energy, and natural bond orbital analyses have been carried out using density functional theory with a B3LYP/6-311++G(d,p) level of the basis set. The vibrational modes have been unambiguously assigned using potential energy distribution analysis. The scaled wavenumbers are in good agreement with the experimental results. Natural bond orbital analysis has confirmed the intermolecular/intramolecular charge transfer interactions. HOMO-LUMO analysis was carried out to explore charge delocalization on the (2*E*)-IPPMP molecule. A molecular docking study has supported the anticonvulsant activity of the title molecule.

1. Introduction

Epilepsy is a rather neurobiological group of disorders. It has multiple origins and aspects depending upon the affected brain areas. It affects nearly 50 million people of the world's population [1–3]. The hydrazinecarboxamide derivatives have a wide spectrum of biological activities. Among these activities are anticancer and antioxidant [4], antifertility [5], antimicrobial [6, 7], anticonvulsant [8, 9], and anti-inflammatory [10] activities. The title molecule (2*E*)-2-[3-(1*H*-imidazol-1-yl)-1-phenyl-propylidene]-*N*-(4-methylphenyl)hydrazinecarboxamide ((2*E*)-IPPMP) was synthesized in our laboratory and its crystal structure was previously reported [11]. (2*E*)-IPPMP exhibited anticonvulsant activity with 83% and 50% seizure protection at a dose level of 718 μmol/kg in subcutaneous pentylenetetrazole (scPTZ) and maximal electroshock seizure (MES) screens, respectively, without any neurotoxicity [9].

Literature screening indicated that computational studies on the (2*E*)-IPPMP molecule have not yet been reported. Therefore, detailed investigations of structural properties and vibrational spectral analysis of the (2*E*)-IPPMP molecule were carried out in the present study using density functional theory (DFT) computations. Moreover, the biological