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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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Abstract

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⋯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.