

Theoretical investigation of physicochemical and biological properties of some imidazole derivatives : a DFT approach and molecular docking analysis

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We present in this work the density functional theory (DFT) calculations of the geometric parameters, electronic structure, reactivity analysis, and spectroscopic properties on Schiff's bases substituted with: $-CH_3$, $-CH_2CH_3$, $-OCH_3$, and $-Cl$ groups in the para position, 2-(4-R-phenyl)-4,5-diphenyl-1H-imidazoles (Imd), Imd1–Imd4 in ethanol solvent. Torsion and dihedral angles scanning elucidate the intramolecular interaction regarding the steric and electronic effects of the substituent on the energetic stability of title compounds. A quantum chemical calculation provides the relationship between corrosion inhibition and molecular reactivity descriptors. Molecular electrostatic potential (MEP) is stimulated for identifying the better reactive sites for electrophilic and nucleophilic attacks. The computation of HOMA and FLU indexes indicates the reduction of aromaticity when going from Imd1 to Imd4 compounds, because of the presence of the chlorobenzene ring, as shown by the HOMA and FLU values of the last compound (HOMA = 0.963 and FLU = 1.013). Imd3 has significant luminescence, given by the value of Stokes shifts (55.33). The calculated linear polarizability and static first-order hyperpolarizability showed that the material exhibited good nonlinear optical behavior and could be used for NLO devices. Drug-likeness and ADME prediction have revealed that all structures presented a good absorption and oral bioavailability. Molecular docking has been used to study the anticancer activity of the investigated molecules against vascular endothelial growth factor receptors (VEGFR-1 and VEGFR-2). All compounds demonstrated high affinity to the active sites of the two protein targets with a binding energy of [8.3–8.8 kcal mol⁻¹] For VEGFR-1 and [10.3–10.9 kcal mol⁻¹] for VEGFR-2. The selected molecules hold strong potential as drug candidate for the development of new anticancer agents.

Key words: Hyperpolarizability, Spectroscopic properties, Corrosion inhibition, NLO, Anticancer activity.