The Innovation Engine of India

Synthesis, characterization, electronic structure, vibrational assignment, HOMO-LUMO, Mulliken charge analysis, docking, antioxidant and anticancer studies of (1-methyl)-2-(2-arylaminothiazol-4-yl)benzimidazole

R L Anashafer[b], S P Selvin Pragalath Paul[b] & T F Abbs Fen Reji*[a]

[a]Department of Chemistry and Research Centre, Nesamony Memorial Christian College, Marthandam 629 165, Tamil Nadu, India

[b]Manonmaniam Sundaranar University, Tirunelveli 627 012, Tamil Nadu, India

E-mail: anashaferborciya@gmail.com

Received 16 August 2023; accepted (revised) 24 January 2024

The compound (1-methyl)-2-(2-arylaminothiazol-4-yl)benzimidazole has been characterized by IR spectra. The theoretical calculations of the mentioned compound have been carried out using the more popular density functional theory method, Beck's-3-parameter-Lee Yang Parr (B3LYP) in 6-31G basic set. Optimized geometries of the molecule have been described and collated with the experimental values. The experimental atomic charges demonstrate adequate concurrence with the theoretical prediction from DFT. Theoretical spectral values have been interpreted and compared with FT-IR spectra. The IR spectra are obtained and assigned by vibrational analysis. The Mulliken population analysis on atomic charges has been computed using DFT calculation. A correlation between the theoretical and the experimental spectra has been achieved. The calculated HOMO and LUMO energy gaps also confirm that charge transfer occurs within the molecule. The compound C2 has highest activity against Hep-C cell line. Five membered heterocyclic moieties have been proved to posses strong biological activities. Hence a series of noval benzimidazolyl thiazoles have been synthesized by multi-step reaction from 2-acetyl benzimidazole and hydroxylamine hydrochloride as starting materials and structure characterized by NMR and mass spectroscopy. The antioxidant activities of the derivatives have been determined by DPPH scavenging assay. The synthesized compounds show remarkable antioxidant activity. They show excellent anticancer activity.

Keywords: Gaussian, DFT, B3LYP, Mulliken charges, HOMO, LUMO, DPPH, Docking, Anti-oxidant, Anticancer

Benzimidazole is an aromatic heterocyclic organic