

Electronic structure, vibrational spectroscopic assignment antioxidant, anticancer activity and DFT study of some novel (1-benzyl)-2-(2-alkylaminothiazol-4-yl)benzimidazole

R L Anashafer^{a,b}, S P Selvin Pragalath Paul^a & T F Abbs Fen Reji^{*a}

^aDepartment of Chemistry and Research Centre,
Nesamony Memorial Christian College, Marthandam 629 165, Tamil Nadu, India

^bManonmaniam Sundaranar University, Tirunelveli 627 012, Tamil Nadu, India

E-mail: abbsfen@gmail.com

Received 25 March 2024; accepted (revised) 27 May 2024

The quantum mechanical calculation of optimized parameters and energies of (1-benzyl)-2-(2-alkylaminothiazol-4-yl)benzimidazole have been done by using Density Functional Theory (DFT) with 6-31G(d,p) basis set. The optimized geometrical parameters acquired by DFT are in better agreement with analogues single experimental data. Electrical dipole moment values have been computed by using *ab initio* and DFT quantum mechanical calculations. The total energy, dipole moment and energy difference are calculated for the derived compounds. The HOMO-LUMO energies have been calculated. Energy gap of HOMO-LUMO strongly supports the presence of intramolecular energy transfer within the molecule. The compound **1a** shows highest activity against Hep-C cell line. The antioxidant study has also evaluated excellent IC₅₀ value. It shows the best inhibitory concentration against breast cancer. The compound (1-benzyl)-2-(2-ethylaminothiazol-4-yl)benzimidazole is found to be highly active on the MDA-MB-231 breast cancer cell line.

Keywords: DFT, Dipole moment, HOMO, LUMO, DPPH, Docking