Experimental, DFT, biological activity and molecular docking studies of 5-ethylsulphonyl-2-phenyl-benzoxazole

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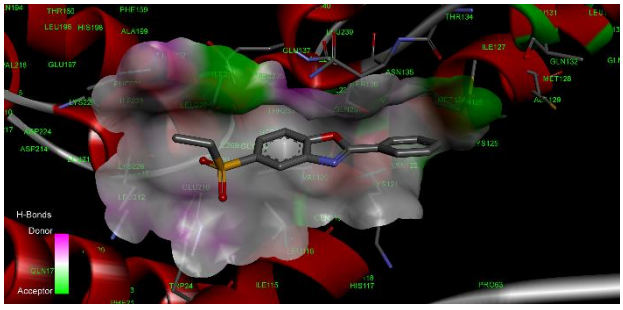
Abstract

Synthesis, optimized molecular structure, vibrational spectroscopic (FT-IR, ^{1}H NMR) investigations, DFT studies (optimized geometry, vibrational band assigned, MEP, NBO analysis, frontier molecular orbitals, NLO effects and thermodynamic functions), antimicrobial activity and molecular docking study of 5-ethylsulphonyl-2-phenyl-benzoxazole have been reported. The DFT calculations have been performed by using Hartree-Fock (HF) and the functional B3LYP and BYLP with 6-311++G(d,p) basis set. The calculated geometrical parameters are in agreement with that of similar derivatives. Predicted vibrational frequencies have been assigned and compared with the experimental IR spectra and they support each other. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. HOMO and LUMO levels have been defined to compare values of HOMO-LUMO gap of the novel benzoxazole derivative that those for using the light-emitting element and the investigated compound. The first order hyperpolarizability of the 5-ethylsulphonyl-2-phenyl-benzoxazole was calculated. Our computational results yield that β_{tot} for the title compound is greater than those of urea. Microbiological results indicated that the title compound possessed a broad spectrum activity against the tested Gram-positive, Gram-negative bacteria. Prediction of Activity Spectra (PASS) analysis of the title compound predicts muscular dystrophy treatment activity as the most probable activity with (probability to be active) value of 0.843. Molecular docking of the title compound with the dystrophin protein exhibited the good binding affinity with energy of −6.3 kcal/mol and having good interaction with amino acids SER-136, TRP-112, LYS-121, VAL 120, MET-124, LEU-116, ASN-135 and GLU-137 for the compound.



Keywords: Benzoxazoles; biological activity; molecular docking; density functional theory; spectroscopy; organic light-emitting diode.