Polycyclic Aromatic Compounds >
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Research Articles

Synthesis, Computational, Antibacterial and Antifungal Investigation of Two Tri-Fluorinated Chalcones of 1-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)ethan-1-one

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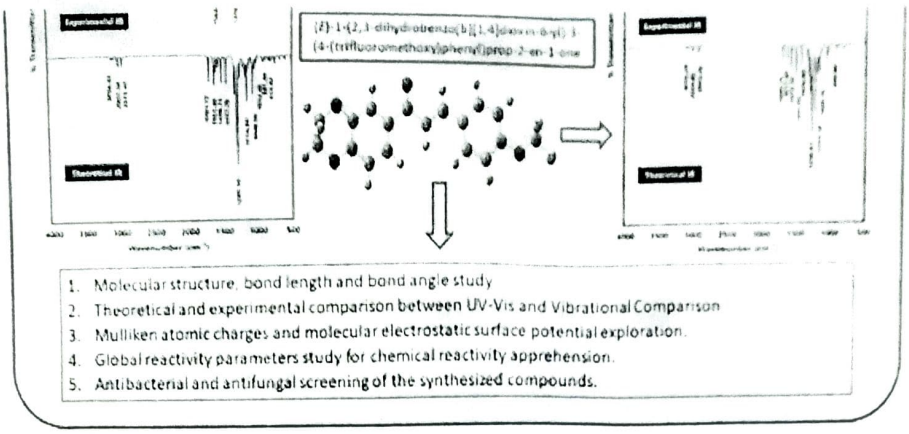
Abstract

In the present study, we report the combined experimental and computational study along with antimicrobial screening of two tri-fluorinated chalcones from 1-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)ethan-1-one. The (*E*)-1-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-3-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (DBTFP-1) and (*E*)-1-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-3-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one (DBTFP-2) were synthesized by the famous Claisen-Schmidt condensation reaction.

and bond angles were performed by using density functional theory (DFT) with a B3LYP functional and 6-31G(d,p) basis set. The electronic properties were computed using Time-Dependent density functional theory (TD-DFT) with a B3LYP functional and 6-31G(d,p) basis set for the optimized geometries. The lower band gap in DBTFP-1 demonstrated the inevitable intramolecular charge transfer. The UV-Visible simulations were performed in the gas phase and dichloromethane (DCM) solvent. The experimental UV-Visible analysis was performed in DCM solvent. The first singlet excited state was attributed to the n-π* and second singlet excited state to the π -π* electronic transition. The scaled vibrational bands of titled compounds were compared with experimental observations and correct vibrational assignments were made. Various global reactivity parameters were analyzed and discussed to apprehend the chemical behavior of the synthesized chalcones. MESP and contour surfaces revealed negative potentials near the oxygen atoms and positive potentials over the hydrogen atoms. Mulliken charge study revealed that C17 and C33 are the most negative and positive carbon atoms in DBTFP-1, respectively, whereas C17 and C35 are the most negative and positive carbon atoms in DBTFP-2. The antibacterial activity was performed against *P. vulgaris* and *S. aureus* and antifungal activity against *A. niger* and *C. albicans*. The antimicrobial activity for these two compounds was correlated with LUMO and band gap energy. The magnificent antimicrobial activity of DBTFP-1 was attributed to its more stabilized LUMO and lower band gap than DBTFP-2.

Synthesis, Computational, Antibacterial



1. Molecular structure, bond length and bond angle study
2. Theoretical and experimental comparison between UV-Vis and Vibrational Comparison
3. Mulliken atomic charges and molecular electrostatic surface potential exploration.
4. Global reactivity parameters study for chemical reactivity apprehension.
5. Antibacterial and antifungal screening of the synthesized compounds.

Keywords: Density functional theory, chalcones, molecular electrostatic potential

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Disclosure statement

No potential conflict of interest was reported by the authors.

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