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Quantum chemical calculations, molecular docking and ADMET studies of *trans*-4-(trifluoromethyl)cinnamic acid

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trans-4-(Trifluoromethyl) cinnamic acid (4TFCA) has a -C=C- double bond among the aromatic system and the carboxyl ring which disturbed the π-electrons of the molecule. The geometrical parameters of 4TFCA is computed using the DFT/B3LYP by higher basis set (6-311++G(d,p)) and the frontier molecular orbital analysis is achieved. FTIR and FT-Raman spectra of 4TFCA have been obtained in the regions 4000-400 cm^{-1} and 4000-50 cm^{-1}. The experimental vibrational frequencies are in good coordination with the calculated wavenumbers. The absorption spectra of 4TFCA have been calculated by using the time dependent/density functional theory approach. The stability of a molecule rising from hyper-conjugative π →π* exchanges and charge delocalization has been calculated using natural bond orbital (NBO) analysis. The thermodynamic and charge responses have been studied. In addition, the results of molecular docking reveal that the molecule 4TFCA has the highest binding energy (–6.10 kcal/mol) with the histone deacetylase inhibitor (HDAC8). To understand the molecule's drug likeness, ADMET analysis has also been studied.

Keywords: DFT, *trans*-4-(Trifluoromethyl)cinnamic acid, Vibrational assignments, Docking, ADMET