Synthesis, Spectroscopic Properties, Quantum Chemical Calculations, and Biological Activities of 2-{[5-(2-Fluorophenyl)-4-(4-methylphenyl)-4*H*-1,2,4-triazol-3-yl]sulfanyl}-1-[3-methyl-3-(2,4,6-trimethylphenyl)-cyclobutyl]ethan-1-one

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Abstract—2-{[5-(2-Fluorophenyl)-4-(4-methylphenyl)-4*H*-1,2,4-triazol-3-yl]sulfanyl}-1-[3-methyl-3-(2,4,6-trimethylphenyl)cyclobutyl]ethanone was synthesized and characterized by spectral techniques and quantum chemical calculations. The molecular geometry, vibrational frequencies, and gauge-including atomic orbital (GIAO) ^{1}H and ^{13}C NMR chemical shifts of the title compound in the ground state were calculated using the density functional method (B3LYP) with the 6-311G(*d*,*p*) basis set, and its electronic absorption spectra were calculated by the TD-DFT method based on the B3LYP/6-311G(*d*,*p*) level optimized structure in ethanol by using the PCM model. The calculated results showed that the optimized geometry well reproduces the theoretical vibrational frequencies, and the calculated chemical shifts were in a good agreement with the experimental values. The energetic behavior of the title compound was examined using the B3LYP method with the 6-311G(*d*,*p*) basis set in the framework of the Onsager and polarizable continuum model (PCM). In addition, DFT calculations of frontier molecular orbitals were carried out at the B3LYP/6-311G(*d*,*p*) level of theory. The title compound showed antibacterial and antioxidant activities at different levels.

Keywords: theoretical calculations, density functional theory, antioxidant activity.

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