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Studies towards investigation of Naphthoquinone-based scaffold with crystal structure as lead for SARS-CoV-19 management

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ABSTRACT

In this work, 1-(4-bromophenyl)-2a,8a-dihydrocyclobuta[*b*]naphthalene-3,8–dione (1-(4-BP)DHCBN-3,8-D) has been characterized by single crystal X-ray to get it's crystal structure with R(all data) - R1 = 0.0569, wR2 = 0.0824, ^{13}C and ^{1}HNMR, as well as UV–Vis and IR spectroscopy. Quantum chemical calculations via DFT were used to predict the compound structural, electronic, and vibrational properties. The molecular geometry of 1-(4-BP)DHCBN-3,8-Dwas optimized utilizing the B3LYP functional at the 6–311++*G*(d,p) level of theory. The Infrared spectrum has been recorded in the range of 4000–550 cm^{-1}. The Potential Energy Distribution (PED) assignments of the vibrational modes were used to determine the geometrical dimensions, energies, and wavenumbers, and to assign basic vibrations. The UV–Vis spectra of the titled compound were recorded in the range of 200-800 nm in ACN and DMSO solvents. Additionally, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap and electronic transitions were determined using TD-DFT calculations, which also simulate the UV–Vis absorption spectrum. Natural Bond Orbital (NBO) analysis can be used to investigate electronic interactions and transfer reactions between donor and acceptor molecules. Temperature-dependent thermodynamic properties were also calculated. To identify the interactions in the crystal structure, Hirshfeld Surface Analysis was also assessed. The Molecular Electrostatic Potential (MEP) and Fukui functions were used to determine the nucleophilic and electrophilic sites. Additionally, the biological activities of 1-(4-BP)DHCBN-3,8-D were done using molecular docking. These results demonstrate a significant therapeutic potential for 1-(4-BP)DHCBN-3,8-D in the management of Covid-19 disorders. Molecular Dynamics Simulation was used to look at the stability of biomolecules.

1. Introduction

Quinones are one of the most explored classes of naturally occurring bioactive molecules isolated from plants and microorganisms playing key pharmacological roles in cancer and inflammation [1]. Moreover, they have also been found effective in managing hepatitis B, cardiovascular, and reproductive disorders [2]. Quinones are 2e^{-} and 2H^{+} acceptors and participate in cellular redox and alkylation reactions to generate reactive oxygen species (ROS) by exhibiting molecular interactions with mitochondrial oxidoreductases such as ubiquinone reductase (NQO1), cytochrome P450 (CYP450), and apoptosis-inducing factor (AIF) [3]. However, their potential use in the management of SARS-CoV-2 has garnered considerable interest recently as the quinone-based scaffolds, such as vitamin K, coenzyme Q10, dexamethasones, and methylprednisolone, have proven effective in managing the progression and increasing the survival rate of the SARS-CoV-19 patients [4]. They

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