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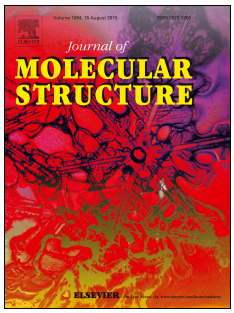

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Microwave-assisted synthesis, structural characterization, DFT studies, antibacterial and antioxidant activity of 2-methyl-4-oxo-1,2,3,4-tetrahydroquinazoline-2-carboxylic acid

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ABSTRACT

In the present study a new tetrahydroquinazoline-2-carboxylic, $C_{10}H_{10}N_2O_3$, **1'**, was synthesized and its structure was characterized by elemental analysis IR, ^{1}H NMR, ^{13}C NMR data and high-resolution mass spectrometry. The spectral results are in line with the proposed structure. Single crystal X-ray structural analysis of the compound show that the crystal structure adopts a monoclinic space group $P2_1/c$, with the packing of the molecule stabilized by C=O……H-O, N-H…….O=C-O- intermolecular hydrogen bonding. The theoretical geometrical parameters of the compound have been calculated using density functional (DFT) and time-dependent density functional (TD-DFT) theory methods and have been used to predict the thermodynamic one-electron redox potential and the electronic absorption property of the compound. The theoretical characterization matched the experimental measurements, showing a good correlation. The calculated HOMO-LUMO gap (4.79 eV) suggests that compound **1'** could be a potential antioxidant. The synthesized compound was screened for its in vitro antimicrobial activity against selected bacterial strains and antioxidant activity using the TAC, FRAP, NO and ABTS models. In vitro antioxidant activity of **1** showed a moderate activity, but weaker scavenging