# Synthesis, Molecular Structure, Spectroscopic analysis, and Biological activities of new 2,4-Dinitrophenylhydrazone derivatives: A combined experimental, and theoretical study

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**Abstract**

The present work focuses on the synthesis and characterization of four hydrazone derivatives. The structures of the synthesized compounds were determined through spectroscopic techniques via., EI MS, &1H NMR. The experimental results demonstrate that the obtained compounds successfully synthesize and screened for DPPH free radical scavenging activity, ferrous ion-chelating activity, ferric ion reducing activity, total antioxidant activity, and hydroxyl radical scavenging activity. Density Functional Theory (DFT) calculations were carried out by the Gaussian 09 package by using a hybrid density functional B3LYP (at 6-31G, 6-311G, and 6-31G++(d,p) basis sets) to investigate the electronic, molecular structures and provide useful spectroscopic and structural information. The computational data obtained from 1H NMR calculations were quite compatible with the experimental results. DFT calculations optimized the molecular geometry and estimated the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy of these compounds. Additionally, the charge transfer within the molecule and favorable sites for the electrophilic and nucleophilic attack was explored. Furthermore, the frontier molecular orbital (FMO) calculations were used to calculate different reactivity parameters, i.e., ionization potential, electron affinity, electronegativity, chemical hardness, chemical softness, and electrophilicity index.

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