

Research Article

Synthesis, and Structural Characterization of (E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono) methyl)phenyl) piperidine: A Combined Spectroscopic and Computational Study

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Abstract

This study Hydrazine-based piperidine derivatives are widely recognized for their significant roles in pharmaceutical development and material science research. In this context, the present study aimed to synthesize a novel hydrazone derivative to explore its structural and electronic features. This study presents the synthesis and structural characterization of (E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono)methyl)phenyl)piperidine (DHP). The compound was obtained through a condensation reaction between 4-(piperidin-1-yl) benzaldehyde and (2,4-dinitrophenyl) hydrazine, achieving an 88% yield. Its structure was confirmed using ¹H NMR, ¹³C NMR, FT-IR, and UV-Vis spectroscopy. Molecular electrostatic potential (MEP) analysis highlighted regions of charge distribution, with electronegative zones concentrated around nitro (-NO₂) groups and electropositive areas near the hydrazone linkage. The UV-Vis spectrum exhibited a peak at 406 nm, attributed to π - π^* transitions and intramolecular charge transfer. The results validate the successful synthesis and structural integrity of DHP, underscoring its significance in organic synthesis, photophysical investigations, and material science.

Keywords: Hydrazine; Electrostatic; Electronegative; Transfer; Photophysical

1. Introduction

The development and structural study of novel organic molecules has been a focal point in medicinal and material chemistry due to their advantageous roles in drug discovery, catalysis, and molecular electronics (Taylor et al., 2016; Guillemard et al., 2021). Among the various

heterocyclic frameworks, piperidine derivatives have garnered considerable interest because of their prevalence in bioactive compounds, including pharmaceuticals, alkaloids, and agrochemicals (Mallappa et al., 2024; Heravi, & Zadsirjan, 2020). These piperidine-based structures have been broadly studied for their diverse pharmacological activities, such as anti-inflammatory, antimicrobial, anticancer, and central nervous system (CNS) modulatory properties (Frolov & Vereshchagin, 2023; Kant et al., 2013). Additionally, hydrazone-based compounds are well known for their wide spectrum of biological actions, including antibacterial, antifungal, antitumor, and antioxidant properties (Tafere et al., 2025; Socea et al., 2022). The fusion of these two structural motifs into a single molecular entity has the potential to yield novel compounds with enhanced biological efficacy and unique structural characteristics.

(E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono)methyl)phenyl)piperidine (DHP) is a newly synthesized compound that incorporates a piperidine framework with a hydrazone linkage and a dinitrophenyl moiety. The hydrazone functional group is especially significant due to its capacity to engage in tautomeric equilibria, metal chelation, and hydrogen bonding, making it an intriguing candidate for applications in medicinal and coordination chemistry (Sathyadevi et al., 2012; Raczuk et al., 2022; Abdulazeez et al., 2018). Additionally, hydrazone derivatives are well comprehended for their various biological actions, including antibacterial, antifungal, antitumor, anti-inflammatory, and antidiabetic properties (de Oliveira Carneiro Brum et al., 2020; Rollas et al., 2007), which widens the scope for the pharmacological investigation of DHP. Furthermore, the dinitrophenyl unit is a strong electron-withdrawing group that can markedly affect the molecule's electronic properties and reactivity. Its existence not only stabilizes the hydrazone connection through resonance and inductive effects but also improves the potential of the molecule to participate in specific non-covalent interactions, such as π - π stacking and charge-transfer, which are applicable in both molecular recognition and supramolecular assembly (Singh et al., 2021; Haque et al., 2023). The piperidine skeleton, a privy structure in medicinal chemistry, is known for its impact on the pharmacokinetic and pharmacodynamic manners of bioactive molecules, enhancing membrane permeability, receptor binding, and metabolic stability (Frolov et al., 2023; Goel et al., 2018; Mitra et al., 2022). The integration of this heterocyclic ring into the DHP structure additionally strengthens its potential for drug-like properties. Therefore, a comprehensive structural investigation of this novel compound is crucial to understanding its potential applications across different scientific fields, including drug design, material science, and catalysis. Thorough characterization not only explains the molecular conformation and

electronic distribution but also furnishes an understanding of intermolecular interactions that could handle its behavior in biological and chemical environments.

This study presents the synthesis and structural characterization of (E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono)methyl)phenyl)piperidine through various spectroscopic techniques. The synthesis follows an efficient condensation reaction between the corresponding piperidine derivative and 2,4-dinitrophenylhydrazine under controlled conditions. The structural features of the compound are elucidated using Fourier-transform infrared (FT-IR) spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy, and mass spectroscopy. These analytical approaches furnish essential understandings of the functional groups, bonding interactions, electronic transitions, and three-dimensional molecular configuration of the synthesized compound.

Spectroscopic techniques play a crucial role in determining the stability, purity, and conformational behavior of novel molecules. FT-IR spectroscopy helps identify characteristic functional groups, while NMR spectroscopy provides a detailed understanding of the electronic environments of hydrogen and carbon atoms within the structure. UV-Vis spectroscopy is useful for analyzing electronic transitions influenced by the presence of the dinitrophenyl group.

The novelty of this research lies in the successful synthesis and structural characterization of an unprecedented piperidine-hydrazone derivative. The comprehensive structural insights gained from this study contribute to fundamental chemical knowledge and open avenues for further exploration of potential biological or material applications of the synthesized molecule. This work emphasizes the importance of designing innovative heterocyclic derivatives with tailored electronic and structural properties, making them promising candidates for future studies in drug design and functional materials.

2. Methods and Materials

Methods

The FT-IR spectrum of (E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono)methyl)phenyl)piperidine (DHP) was recorded at 25 °C using a Perkin-Elmer FT-IR spectrometer to identify the molecule's functional groups and vibrational characteristics. Structural analysis of carbon and hydrogen atoms was carried out through ^{13}C and ^1H NMR spectroscopy using a Bruker AVANCE-III spectrometer. The compound's electronic absorption properties were examined via UV-Vis spectroscopy on a Perkin-Elmer Lambda 35 spectrometer, covering the 200–600 nm range with a 1 nm bandwidth.

Materials

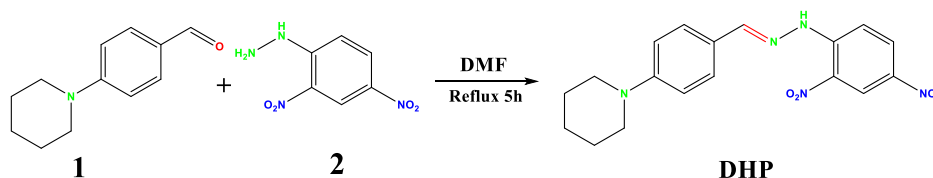
All chemicals required for the synthesis of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine (DHP) were obtained from Sigma-Aldrich and used directly in the reaction without any further purification.

Computational details

DFT computations were performed utilizing the Gaussian 09 software (Frisch, 2009), employing the B3LYP functional combined with the 6-311++G(d,p) basis set (Jamal et al., 2024; Murugavel et al., 2019). This approach was used to investigate various properties of the designed molecule, E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono)methyl)phenyl)piperidine (DHP), as illustrated in Figure 1.

3. Result and Discussion

Synthesis of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine (DHP)



Scheme 1

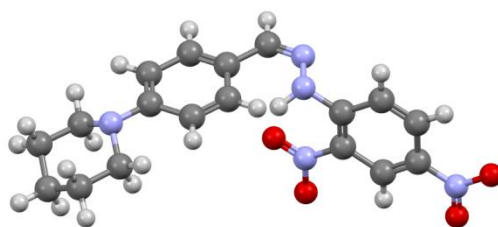


Figure 1. Structure of (E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono)methyl)phenyl)piperidine (DHP)

The DHP was synthesized by reacting 4-(piperidin-1-yl)benzaldehyde (1) with (2,4-dinitrophenyl)hydrazine (2), as shown in Scheme 1. According to the literature (Jamal et al., 2024; 2025; Medeiros et al., 2023), Initially, 0.50 g (2.64 mmol) of (2,4-dinitrophenyl)hydrazine was dissolved in 20 mL of DMF, followed by the addition of 0.52 g (2.62 mmol) of 4-(piperidin-1-yl)benzaldehyde. The reaction mixture was then refluxed for 5 hours, during which a pale yellow

precipitate gradually formed as the solution volume reduced to 10 mL. The precipitate was collected by filtration and purified by sequential washing with 5 mL of cold methanol and 10 mL of hexane. The solid product was then recrystallized from methanol and dried under vacuum. The final DHP product was obtained as a yellow solid with a yield of 88%, equivalent to 0.90 g. However, the structural representation of DHP is depicted in Figure 1.

NMR study

The ^1H NMR spectrum (Figure 2) of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine), recorded in DMSO-d_6 , exhibits well-defined chemical shifts that are consistent with the expected structural features and comparable to similar reported compounds. In the downfield region (9.0–8.0 ppm), three distinct peaks are observed, including a noticeably broad resonance attributed to the hydrazone proton ($-\text{C}=\text{NNH}$) and the aromatic protons of the 2,4-dinitrophenyl moiety. The deshielding of these signals is characteristic of the electron-withdrawing influence of nitro ($-\text{NO}_2$) substituents, which has been similarly reported for hydrazone derivatives bearing nitro-substituted aromatic rings (Pretsch et al., 2000; Pavia et al., 2015). Typically, the hydrazone proton appears between 8.5–9.2 ppm in such systems, consistent with the observed values. In the 8.0–6.7 ppm region, three broad peaks are present, corresponding to aromatic protons of both the phenyl (benzyl) and the dinitrophenyl rings.

The mild broadness of these signals suggests conformational flexibility or electron delocalization effects, which is in agreement with earlier observations for aromatic hydrazones incorporating nitro-substituted phenyl groups (Pavia et al., 2015; Pretsch et al., 2013; Sasaki., 1985). Aromatic proton signals for similar systems generally appear in the 7.0–8.5 ppm range. Moving to the 4.0–3.0 ppm region, two signals are noted, one of which appears as a tall, broad peak. These are assigned to the methylene ($-\text{CH}_2-$) protons of the piperidine ring, particularly those adjacent to the phenyl ring, and potentially to benzylic protons in proximity to the imine linkage ($-\text{CH}=\text{N}$). The chemical shift and broadness are in agreement with literature reports for hydrazone derivatives containing piperidine-linked aromatic systems, where aliphatic $-\text{CH}_2$ protons adjacent to electron-withdrawing groups are typically observed around 3.1–4.0 ppm (Sharma, 2007; Pavia et al., 2015; Pretsch et al., 2013; Sasaki., 1985). Finally, a broad resonance in the 2.0–1.0 ppm region is attributed to the remaining aliphatic protons of the piperidine ring, which are shielded within the saturated cyclic environment. This is consistent with reported piperidine derivatives, where ring methylene protons generally resonate between 1.2–2.5 ppm depending on substitution (Field et al., 2013; Pavia et al., 2015; Sasaki., 1985; Pouchert et al., 1993).

The overall spectral pattern — featuring deshielded aromatic resonances, broad hydrazone-associated signals, and well-defined aliphatic peaks — provides clear confirmation of the proposed structure. The recorded chemical shifts and splitting patterns are in good agreement with previously reported hydrazone frameworks and piperidine-based compounds, supporting the successful synthesis and structural integrity of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine).

The ^{13}C NMR spectrum (Figure 2) of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine) recorded in DMSO-d_6 exhibits characteristic peaks that are in excellent agreement with the expected chemical environments in the molecular framework. In the downfield region between 157–140 ppm, three different peaks are observed, which can be assigned to the highly deshielded carbons of the 2,4-dinitrophenyl moiety and the imine ($\text{C}=\text{NNH}$) carbon. The strong electron-withdrawing nature of the nitro ($-\text{NO}_2$) substituents significantly influences the deshielding of carbons located ortho and para to these groups, which typically resonate within the 155–145 ppm range, as documented in related hydrazone derivatives (Pouchert et al., 1993; Field et al., 2013; Pavia et al., 2015; Pretsch et al., 2013; Jamal et al., 2025). The imine carbon is also known to appear around 150–145 ppm [3], supporting this assignment. In the chemical shift range of 140–130 ppm, two peaks are detected, corresponding to quaternary aromatic carbons within the dinitrophenyl and benzyl moieties. Literature reports for hydrazone-linked aromatic systems indicate that quaternary carbons adjacent to substituents usually resonate between 140 and 132 ppm (Stothers, 2012; Pouchert et al., 1993; Field et al., 2013; Pavia et al., 2015; Pretsch et al., 2013), confirming the structural assignment. The 130–120 ppm region reveals three peaks, which can be confidently attributed to the protonated aromatic carbons of both the phenyl and dinitrophenyl rings, an assignment consistent with substituted benzene derivatives (Stothers, 2012; Sharma, 2007; Pavia et al., 2015; Pretsch et al., 2013). Additional signals appearing in the 120–110 ppm window are characteristic of aromatic carbons located near varying electronic environments, such as electron-withdrawing or electron-donating groups, and the observed two peaks in this range are in line with prior reports for structurally similar nitro-substituted hydrazones (Stothers, 2012; Pretsch et al., 2000; Pavia et al., 2015).

A well-defined signal at 55 ppm is observed, which corresponds to the tertiary carbon (C-N linkage) of the piperidine ring. Typically, this carbon resonates between 53–58 ppm in piperidine derivatives, particularly those substituted at the nitrogen, as supported by the literature (Pavia et al., 2015; Pretsch et al., 2013). In the 30–20 ppm region, two peaks are recorded, which can be attributed to the aliphatic methylene ($-\text{CH}_2$) groups of the piperidine

moiety. Such carbons generally appear in the 28–23 ppm range for cyclic amines, depending on the substitution pattern and solvent (Stothers, 2012; Sharma, 2007; Pavia et al., 2015; Pretsch et al., 2013; Field et al., 2013). The overall distribution of peaks across both the downfield aromatic and upfield aliphatic regions not only matches the theoretical expectations but also shows excellent correlation with reported chemical shift values for structurally related hydrazone and piperidine-based compounds. These observations strongly confirm the successful synthesis and structural integrity of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine).

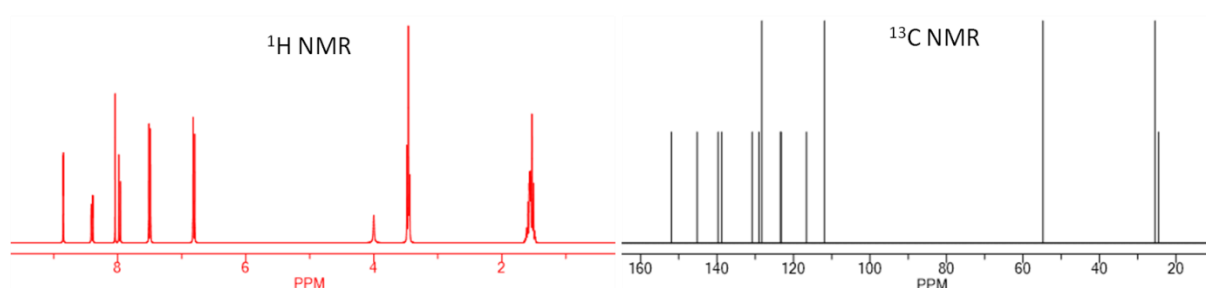


Figure 2. NMR of DHP

FT-IR investigation

The FT-IR spectrum (Figure 3) of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine)/DHP offers a detailed insight into its molecular structure by identifying distinct vibrational modes of its key functional groups. This analysis plays a vital role in verifying the successful synthesis of the compound and confirming its structural authenticity. A significant absorption band observed between 1600 and 1650 cm^{-1} corresponds to the C=N stretching vibration of the hydrazone ($-\text{C}=\text{NNH}-$) group, confirming the formation of the Schiff base bond between the piperidine-substituted benzaldehyde and the dinitrophenyl hydrazine moiety (Sharma, 2007; Pavia et al., 2015; Socrates, 2004; Jamal et al., 2024). Additionally, a broad N-H stretching vibration appearing in the 3200–3400 cm^{-1} range suggests the presence of the secondary amine ($-\text{NH}$) group within the hydrazone framework (Pavia et al., 2015; Socrates, 2004; Jamal et al., 2024).

The broad nature of this peak implies possible intermolecular hydrogen bonding, which may lead to molecular aggregation or dimerization in the solid state. The presence of aromatic benzene rings is confirmed by C-H stretching vibrations observed in the 3050–3100 cm^{-1} range, characteristic of sp^2 hybridized carbon-hydrogen bonds (Sharma, 2007; Pavia et al.,

2015; Socrates, 2004). Additionally, C=C stretching vibrations of benzene rings appear within $1400\text{--}1600\text{ cm}^{-1}$, indicating the presence of conjugated aromatic systems (Pavia et al., 2015; Socrates, 2004). These peaks further confirm the successful incorporation of both the piperidine-substituted benzaldehyde and the 2,4-dinitrophenyl units within the molecular structure. The electron-withdrawing nitro ($-\text{NO}_2$) groups exert a notable influence on the compound's electronic properties. Their presence is distinctly marked by two stretching vibrations: the asymmetric stretching mode appears within $1520\text{--}1570\text{ cm}^{-1}$, whereas the symmetric stretching vibration is observed in the $1300\text{--}1350\text{ cm}^{-1}$ range (Sharma, 2007; Pavia et al., 2015; Socrates, 2004). The significant intensity of these peaks provides strong evidence for the successful incorporation of the 2,4-dinitrophenyl unit, which alters the electronic environment of the molecule. The piperidine ring, a six-membered heterocyclic system, is specified through C-N stretching vibrations in the $1100\text{--}1250\text{ cm}^{-1}$ range, ensuring the presence of this moiety (Pavia et al., 2015; Socrates, 2004). This functional group contributes to the overall stability and reactivity of the molecule. Additionally, the C-H bending vibrations of the piperidine ring are recorded between 1350 and 1450 cm^{-1} (Sharma, 2007; Pavia et al., 2015; Socrates, 2004), further supporting the structural integrity of this component.

The fingerprint region ($600\text{--}900\text{ cm}^{-1}$) of the spectrum contains various absorption bands associated with out-of-plane C-H bending vibrations of substituted benzene rings. These peaks help distinguish different aromatic substitution patterns and further confirm the structural composition. Overall, the FT-IR spectrum of (E)-1-(4-((2-(2,4-Dinitrophenyl)hydrazono)methyl)phenyl)piperidine confirms the presence of all anticipated functional groups, such as hydrazone ($-\text{C}=\text{N}-\text{NH}-$), nitro ($-\text{NO}_2$), aromatic benzene rings, and the piperidine moiety. The clear and well-defined absorption bands corresponding to these groups verify the successful synthesis and molecular structure of the compound. The presence of a distinct C=N stretching band, strong NO_2 asymmetric and symmetric stretching vibrations, prominent C-H and C=C stretching modes, and characteristic C-N vibrations of the piperidine ring collectively validate the structural integrity and purity of the synthesized compound. This FT-IR investigation serves as an essential tool for affirming the formation of the molecule and highlights its potential for further applications in the fields of chemical and pharmaceutical research.

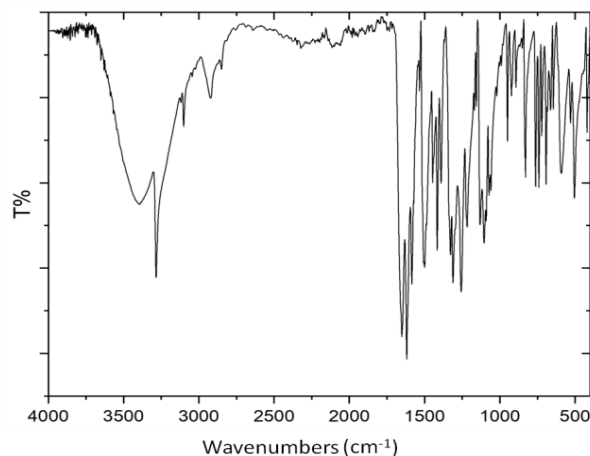


Figure 3. IR of DHP

UV-Vis study

The UV-Vis spectroscopic investigation of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine)/DHP was performed over the 200–700 nm spectral range, identifying a notable absorption peak at 406 nm. This peak corresponds to π - π^* electronic transitions within the conjugated π -system, confirming the molecule's extensive delocalized electron network (Sharma, 2007; Pavia et al., 2015; Pretsch et al., 2013). The presence of the hydrazone ($-\text{C}=\text{N}-\text{NH}-$) functional group plays a crucial role in facilitating electron delocalization, allowing charge distribution between the piperidine-substituted benzene ring and the electron-deficient dinitrophenyl moiety, thereby enhancing intramolecular charge transfer (ICT) characteristics (Pavia et al., 2015; Pretsch et al., 2013). The 2,4-dinitrophenyl fragment, featuring electron-withdrawing nitro ($-\text{NO}_2$) groups, particularly affects the molecule's electronic properties. These nitro groups exert strong inductive and resonance effects, effectively lowering the energy gap between the ground and excited states. As a consequence, a bathochromic shift (red shift) is observed in the absorption spectrum, indicative of enhanced charge separation and stabilization of the excited state (Sharma, 2007; Pavia et al., 2015; Pretsch et al., 2013). Additionally, solvent polarity can influence spectral behavior through solvatochromic effects, wherein highly polar solvents further stabilize the charge-transfer state, leading to variations in absorption wavelength. The noticed absorption at 406 nm confirms the molecule's extended conjugation, making it a promising candidate for applications in organic electronics, semiconductors, and dye chemistry (Pavia et al., 2015; Pretsch et al., 2013). However, the UV-Vis spectrum of DHP is illustrated in Figure 3. Overall, the UV-Vis spectral characteristics of this compound underscore its efficient light absorption, attributed to the hydrazone linkage and nitro substituents. This structural arrangement

enriches its potential utility in pharmaceutical research, materials science, and optoelectronic applications, strengthening its relevance in photophysical and photochemical studies.

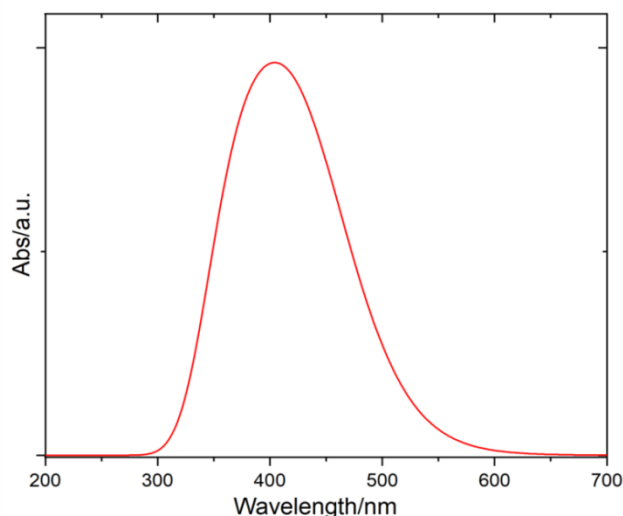


Figure 4. UV-Vis of DHP

FMO analysis

The frontier molecular orbital (FMO) analysis of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine)/DHP offers valuable insights into its electronic characteristics, stability, and potential reactivity. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) play vital roles in confining the molecule's capability to donate and accept electrons, respectively (Jamal et al., 2024; 2025). These orbitals directly influence the compound's chemical behavior, optoelectronic response, and charge transfer capabilities (Jamal et al., 2024; 2024; 2025; Ali et al., 2021). The computed HOMO energy is -5.071 eV, while the LUMO energy is -2.011 eV, resulting in a HOMO-LUMO energy gap of 3.061 eV. This moderate energy gap implies that the compound holds a balance between electronic stability and reactivity, making it a potential candidate for applications in optoelectronic devices and photochemical processes. A smaller energy gap enriches the feasibility of electron excitation, permitting easier transitions between the ground and excited states (Jamal et al., 2024; 2025; Ali et al., 2021). The HOMO is primarily localized over the electron-donating benzylidene-piperidine segment, highlighting its significance in donating electrons during charge transfer interactions. In contrast, the LUMO is concentrated over the electron-deficient 2,4-dinitrophenyl unit, indicating its ability to accept electrons efficiently. This electronic delocalization across the molecule confirms the presence of intramolecular charge transfer (ICT) (Murugavel et al., 2019; Jamal et al., 2024; Pavia et al., 2015; Pretsch

et al., 2013), in which electron density migrates from the electron-rich piperidine-substituted benzylidene unit toward the electron-deficient nitro-substituted phenyl moiety. The existence of nitro ($-\text{NO}_2$) functional groups significantly affects the molecular orbital energies by lowering the LUMO energy, thereby stabilizing the charge-separated excited state (Medeiros et al., 2023; Jamal et al., 2024; 2025; Ali et al., 2021). This electronic modulation contributes to strong absorption characteristics in the visible region, as observed in UV-Vis spectroscopy (Murugavel et al., 2019; Jamal et al., 2024; Pavia et al., 2015). The charge-transfer behavior associated with this molecular framework increases its reactivity and may lead to potential applications in organic electronics, nonlinear optical (NLO) materials, and photovoltaic systems (Ali et al., 2021; Murugavel et al., 2019; Jamal et al., 2024; Pavia et al., 2015; Pretsch et al., 2013). The molecular design, featuring a conjugated π -electron system, makes it a promising material for semiconducting devices, light-harvesting applications, and pharmaceutical research (Medeiros et al., 2023; Jamal et al., 2024; 2024; 2025; Ali et al., 2021). Overall, the FMO analysis underscores the molecular stability, charge-transfer efficiency, and electronic adaptability of this compound. The moderate HOMO-LUMO energy gap, along with efficient electron delocalization, signifies that this molecule can be explored for advanced optoelectronic and semiconductor applications, potentially serving as an effective component in light-responsive materials and electronic sensors. Figure 5 illustrates the FMO diagram for DHP.

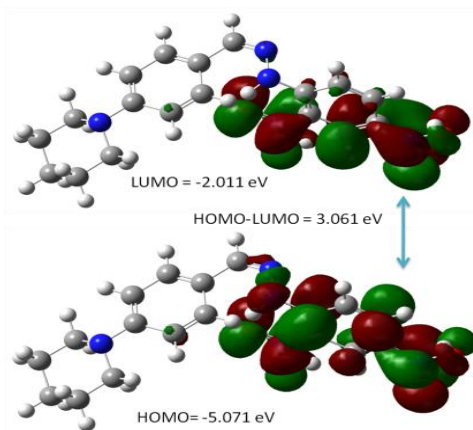


Figure 5. FMO of DHP

Molecular Electrostatic Potential (MEP) Analysis

The MEP surface (Figure 6) of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl) phenyl) piperidine was analyzed within the potential range of $-6.755\text{e}2$ to $6.755\text{e}2$ a.u. to evaluate charge distribution. The yellow region, which partially overlaps with the 4-(piperidin-1-yl)

benzaldehyde moiety, represents a moderate electrostatic potential, implying weak electrostatic interactions (Medeiros et al., 2023; Jamal et al., 2024; 2024; 2025). The blue region, partially covering the (2,4-dinitrophenyl) hydrazine segment, denotes an electropositive nature influenced by the electron-withdrawing nitro groups. The most electronegative zones (red) are focused near the oxygen atoms of the nitro groups, implying their involvement in hydrogen bonding or nucleophilic interactions. The electropositive zones (blue) demonstrate possible locations for electrophilic reactions (Jamal et al., 2024; 2025). This MEP analysis furnishes an understanding of the molecule's reactive centers, which play a key role in its interactions with the chemical and biological systems.

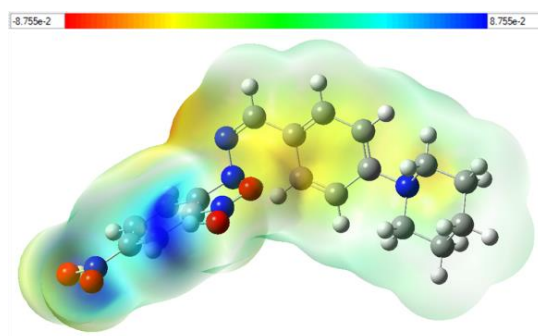


Figure 6. MEP of DHP

4. Conclusion

The synthesis and structural characterization of (E)-1-(4-((2-(2,4-Dinitrophenyl) hydrazono) methyl)phenyl) piperidine (DHP) were successfully performed using NMR, FT-IR, and UV-Vis spectroscopy, which confirmed the expected structural features, particularly the hydrazone and nitro functionalities. The UV-Vis absorption at 406 nm, along with MEP and HOMO-LUMO (3.061 eV) analyses, highlights the significant charge-transfer characteristics and electronic stability of DHP, which are consistent with similar observations reported for other hydrazone-based compounds in previous research. Compared to previous studies, this work presents a new structural framework by incorporating the hydrazone moiety with both a piperidine core and a dinitrophenyl substituent. This fusion significantly affects the electronic distribution, which could play a critical role in tuning the physicochemical and reactive behavior of the molecule. The analysis contributes to the growing understanding of hydrazone derivatives by demonstrating how structural modifications affect electronic and stability profiles, proposing potential applications in material design and drug discovery. However, the study is limited to

structural and theoretical insights, and future work should explore its functional and biological potential to fully assess its practical relevance.

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