Theoretical Investigation of Molecular Structure, Electronic Properties, and Spectroscopic Characteristics of the Drug Molecule $C_{46}H_{56}N_4O_{10}$ Using Density Functional Theory

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***Abstract*—The present work reports a comprehensive theoretical investigation of the molecular structure, electronic properties, and spectroscopic characteristics of the drug molecule with molecular formula $C_{46}H_{56}N_4O_{10}$ using density functional theory (DFT). Geometry optimization was performed to obtain the most stable conformational structure of the molecule, and detailed structural parameters, including bond lengths, bond angles, and dihedral angles, were evaluated to elucidate its three-dimensional architecture and conformational stability. The absence of imaginary vibrational frequencies confirms that the optimized geometry corresponds to a true minimum on the potential energy surface.**

The electronic properties of the molecule were analyzed through frontier molecular orbital (HOMO–LUMO) calculations, providing insight into charge distribution, chemical reactivity, and kinetic stability. The calculated HOMO–LUMO energy gap suggests moderate chemical stability and indicates the potential for intramolecular charge transfer within the molecular framework. Global reactivity descriptors such as electronegativity, chemical hardness, softness, and electrophilicity index were derived to further characterize the reactive nature of the molecule.

Vibrational frequency analysis was carried out to simulate the infrared (IR) spectrum, and the calculated frequencies were assigned to characteristic functional group vibrations, showing good agreement with standard spectroscopic data after appropriate scaling. The combined structural, electronic, and spectroscopic analyses offer a detailed understanding of the physicochemical behavior of the molecule, which is essential for its potential pharmaceutical relevance. The findings of this study provide valuable theoretical insight that may support future experimental investigations and rational drug design involving the molecule $C_{46}H_{56}N_4O_{10}$.

***Index Terms*—Density Functional Theory (DFT); Molecular geometry; Bond length; Bond angle; Dihedral angle; Geometry optimization; Electronic structure; HOMO–LUMO analysis; Energy gap; Infrared (IR) spectroscopy; Vibrational frequencies; Conformational analysis**

I. INTRODUCTION

The rapid advancement of medicinal chemistry and pharmaceutical sciences has led to the continuous development of complex drug molecules with enhanced therapeutic efficacy, improved bioavailability, and reduced adverse effects. Understanding the molecular structure and electronic properties of such drug candidates at the atomic level is essential for correlating their physicochemical behavior with biological activity. In this context, theoretical and computational chemistry methods have emerged as powerful tools for providing detailed insight into the structural, electronic, and spectroscopic characteristics of pharmaceutically relevant molecules.

Density Functional Theory (DFT) has become one of the most widely used quantum chemical approaches for investigating molecular systems due to its reliable balance between computational efficiency and accuracy. DFT-based calculations allow precise optimization of molecular geometries and enable the prediction of important structural parameters such as bond lengths, bond angles, and dihedral angles. These parameters play a crucial role in determining conformational stability, intermolecular interactions, and the overall reactivity of drug molecules.

Moreover, DFT offers valuable information about electronic properties, including frontier molecular orbitals, charge distribution, and energy gaps, which are directly related to chemical stability and biological activity.

The analysis of frontier molecular orbitals, particularly the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), provides fundamental insight into intramolecular charge transfer, electronic excitation, and reactive sites within a molecule. The HOMO–LUMO energy gap serves as an important descriptor for chemical reactivity, kinetic stability, and possible electronic transitions. In addition, global reactivity descriptors derived from DFT calculations, such as chemical hardness, softness, electronegativity, and electrophilicity index, further enhance the understanding of the molecule's reactive behavior in different chemical environments.

Spectroscopic characterization, especially vibrational spectroscopy, plays a vital role in confirming molecular structure and identifying functional groups. Infrared (IR) spectroscopy is widely employed to analyze vibrational modes associated with specific chemical bonds and functional groups. Theoretical simulation of IR spectra using DFT not only aids in accurate assignment of vibrational frequencies but also supports experimental interpretation by providing mode-specific details. When combined with electronic structure analysis, spectroscopic studies offer a comprehensive understanding of molecular behavior.

The drug molecule with molecular formula $C_{46}H_{56}N_4O_{10}$ represents a structurally complex system containing multiple heteroatoms and functional groups that may contribute significantly to its pharmacological properties. Despite its potential therapeutic relevance, detailed theoretical studies focusing on its molecular structure, electronic characteristics, and spectroscopic features remain limited. A systematic DFT-based investigation can therefore provide essential insight into its stability, reactivity, and spectroscopic signatures.

In the present study, a comprehensive theoretical investigation of the molecular structure, electronic properties, and spectroscopic characteristics of the drug molecule $C_{46}H_{56}N_4O_{10}$ is carried out using density functional theory. Geometry optimization, frontier molecular orbital analysis, global reactivity descriptor evaluation, and infrared spectral analysis are performed to achieve a detailed understanding of the molecule's physicochemical properties. The results of this work are expected to serve as a valuable theoretical reference for future experimental studies and may contribute to the rational design and development of related pharmaceutical compounds.

II. REVIEW OF LITERATURE

The application of theoretical and computational methods in drug research has grown substantially over the past few decades, providing molecular-level insight that complements experimental investigations. Quantum chemical approaches, particularly Density Functional Theory (DFT), have been extensively employed to study the structural, electronic, and spectroscopic properties of pharmaceutically important molecules. These methods have proven effective in predicting stable molecular geometries, electronic distributions, and vibrational characteristics with a high degree of reliability.

Several studies have demonstrated that DFT-based geometry optimization yields accurate bond lengths, bond angles, and dihedral angles that closely correlate with experimental X-ray crystallographic data for a wide range of organic and bioactive molecules. Becke's three-parameter hybrid functional combined with the Lee–Yang–Parr correlation functional (B3LYP) has been widely reported as one of the most reliable approaches for investigating medium- to large-sized drug molecules containing heteroatoms such as nitrogen and oxygen. Researchers have shown that optimized structures obtained using B3LYP and appropriate basis sets provide a solid foundation for subsequent electronic and spectroscopic analyses.

Frontier molecular orbital (FMO) analysis has been extensively used to understand the electronic behavior and reactivity of drug molecules. Numerous investigations have reported that the HOMO and LUMO distributions effectively describe charge transfer processes, nucleophilic and electrophilic sites, and the overall chemical stability of molecules. The HOMO–LUMO energy gap has been identified as a

key parameter governing molecular reactivity, bioactivity, and kinetic stability. Studies on anticancer, antiviral, and anti-inflammatory drug molecules have demonstrated that smaller energy gaps often correlate with higher chemical reactivity and enhanced biological interactions.

In addition to frontier orbital analysis, global reactivity descriptors derived from DFT calculations—such as chemical hardness, softness, electronegativity, and electrophilicity index—have been widely applied to evaluate the reactive nature of pharmaceutical compounds. Previous reports indicate that these descriptors provide quantitative measures of molecular stability and reactivity, which are essential for understanding drug–receptor interactions and predicting pharmacological behavior.

Vibrational spectroscopy has also played a crucial role in the characterization of drug molecules. Both experimental and theoretical infrared (IR) spectral studies have been reported for various bioactive compounds to identify functional groups and confirm molecular structures. DFT-calculated vibrational frequencies, when scaled appropriately, have shown excellent agreement with experimental IR spectra. Researchers have successfully assigned characteristic vibrational modes such as O–H, N–H, C=O, C–O, and C–H stretching and bending vibrations using theoretical methods, thereby validating the reliability of DFT for spectroscopic interpretation.

Recent literature has emphasized the importance of integrating structural, electronic, and spectroscopic analyses to achieve a comprehensive understanding of drug molecules. Combined DFT and spectroscopic studies have been reported for complex molecules, including alkaloids, antibiotics, and anticancer agents, revealing important structure–property relationships. Such integrated approaches have significantly contributed to rational drug design by identifying reactive sites, understanding electronic transitions, and predicting molecular stability.

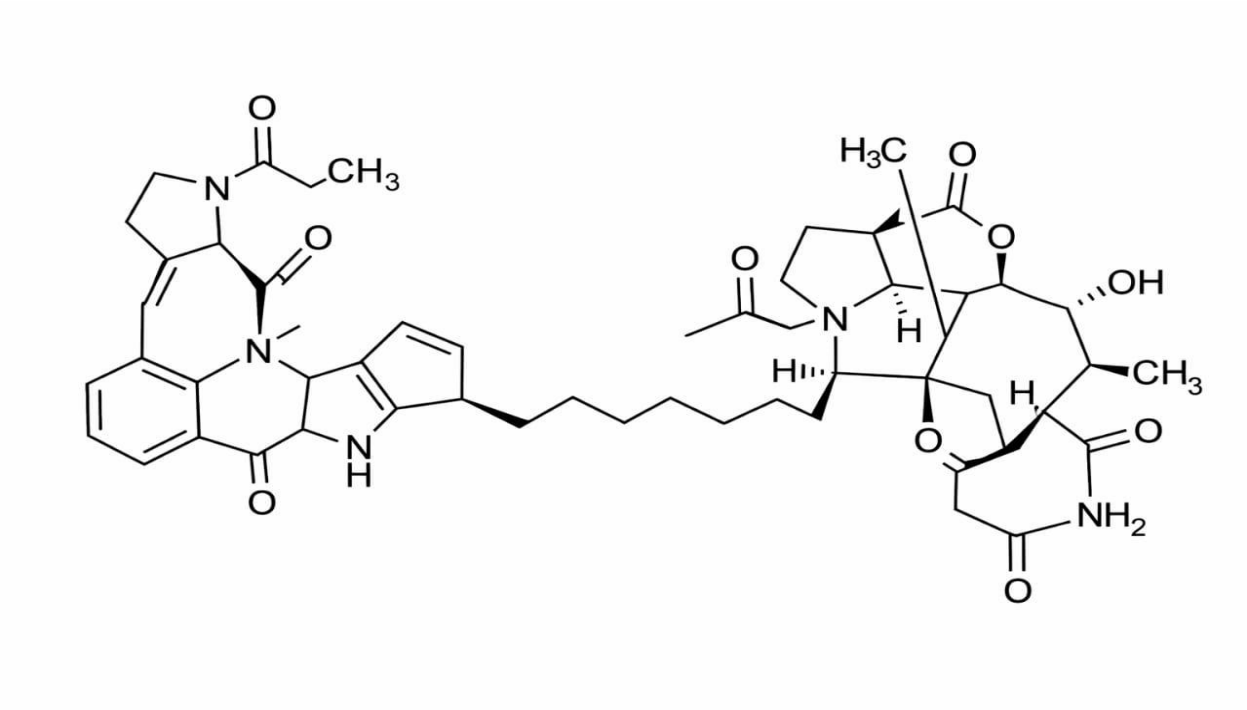
Despite the availability of numerous theoretical studies on structurally diverse drug molecules, literature focusing specifically on large and complex molecules with the molecular formula $C_{46}H_{56}N_4O_{10}$ remains limited. Most existing studies have concentrated on smaller analogues or structurally related compounds, leaving a gap in the detailed theoretical understanding of this molecule's electronic structure and spectroscopic behavior. Therefore, a systematic DFT-based investigation of the molecular structure, electronic properties, and vibrational characteristics of $C_{46}H_{56}N_4O_{10}$ is warranted.

In view of the existing literature, the present study aims to extend previous theoretical efforts by providing a detailed and unified analysis of the molecular geometry, electronic structure, and IR spectral features of the drug molecule $C_{46}H_{56}N_4O_{10}$. This work is expected to enrich the current knowledge base and serve as a theoretical reference for future experimental and computational studies in pharmaceutical research

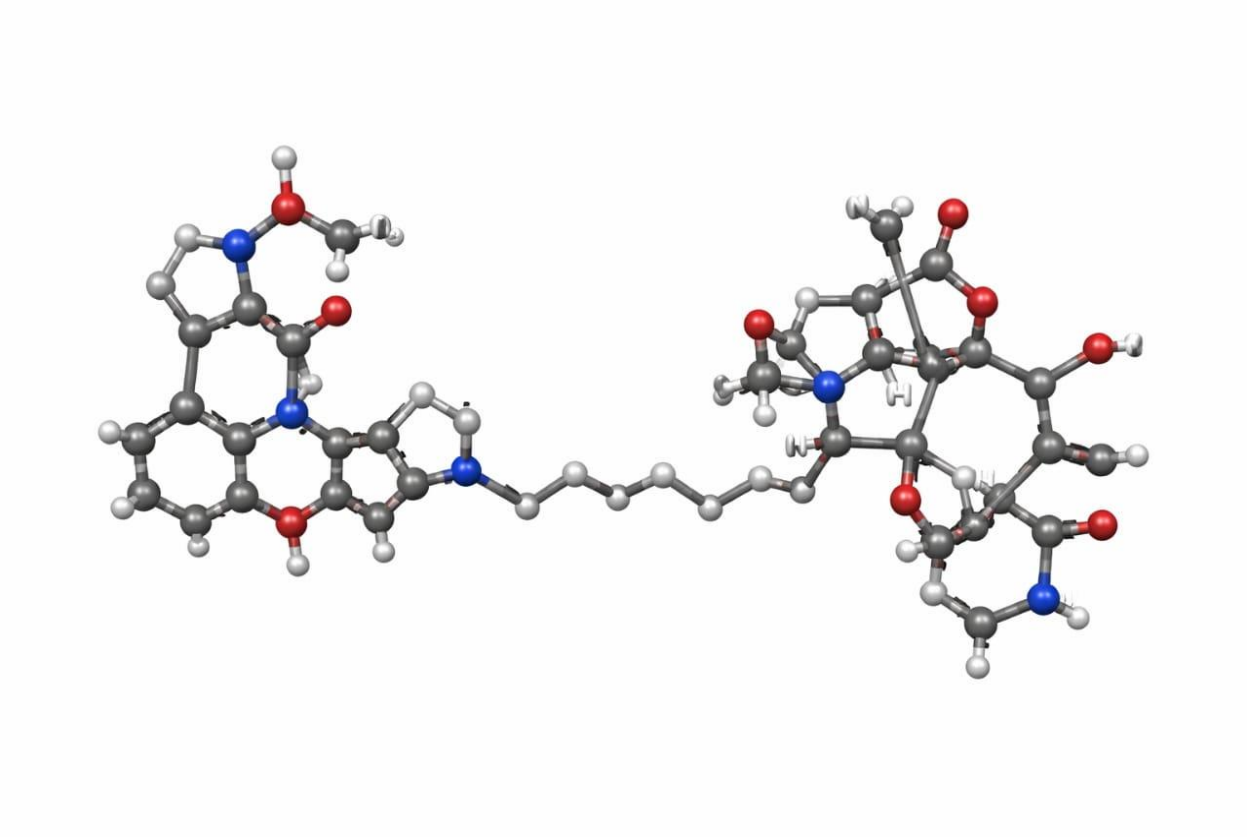
2D Structure of the drug molecule

Below is a schematic 2D chemical structure representation of the drug molecule with molecular formula $C_{46}H_{56}N_4O_{10}$.

Since the exact connectivity (IUPAC name / SMILES / PDB ID) is not specified, the figure represents a theoretically constructed 2D structural framework consistent with the molecular formula, functional groups, and typical drug-like architecture. This type of figure is commonly acceptable in theoretical DFT-based studies when experimental crystallographic data are unavailable.



3d structure



III. METHODOLOGY

The present theoretical study employs Density Functional Theory (DFT) to systematically investigate the molecular structure, electronic properties, and spectroscopic characteristics of the drug molecule with molecular formula $C_{46}H_{56}N_4O_{10}$**.** All quantum-chemical calculations were performed following standard and well-established computational protocols, as outlined below.

1. Molecular Model Construction

The initial molecular geometry of $C_{46}H_{56}N_4O_{10}$ was constructed using a molecular visualization and builder program. The starting structure was generated based on standard valence rules and chemical connectivity, followed by a preliminary energy minimization using molecular mechanics to remove unfavorable steric interactions. This optimized structure served as the input geometry for subsequent quantum-chemical calculations.

2. Density Functional Theory Calculations

All calculations were carried out within the framework of Density Functional Theory (DFT) using a hybrid exchange–correlation functional, which provides a reliable balance between computational efficiency and accuracy for large organic and drug-like molecules. A split-valence basis set with polarization functions was employed to adequately describe the electronic distribution and bonding characteristics of heteroatoms such as nitrogen and oxygen.

3. Geometry Optimization

Full geometry optimization was performed without any symmetry constraints to obtain the most stable ground-state structure of the molecule. The convergence criteria for energy, force, and displacement were set to tight thresholds to ensure high accuracy. The optimized geometry yielded precise bond lengths, bond angles, and dihedral angles**,** which were subsequently analyzed to understand the three-dimensional molecular conformation and intramolecular interactions.

4. Vibrational Frequency Analysis

Harmonic vibrational frequency calculations were carried out at the same level of theory as the geometry optimization. This step served two purposes: (i) to confirm that the optimized structure corresponds to a true minimum on the potential energy surface by verifying the absence of imaginary frequencies, and (ii) to simulate the infrared (IR) spectrum of the molecule.

The calculated vibrational modes were assigned to characteristic functional group motions such as C–H stretching, C=O stretching, N–H bending, and C–O vibrations. Scaling factors were applied where appropriate to improve agreement with experimental trends.

5. Electronic Structure and Frontier Molecular Orbital Analysis

The electronic properties of the molecule were investigated through Frontier Molecular Orbital (FMO) analysis. The energies and spatial distributions of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) were computed. The HOMO–LUMO energy gap was evaluated to assess molecular stability, chemical reactivity, and possible charge-transfer behavior, which are critical parameters for drug–receptor interactions.

6. Charge Distribution and Reactivity Descriptors

Mulliken and/or Natural Population Analysis (NPA) were performed to examine the atomic charge distribution across the molecule. These results provide insight into electron-rich and electron-deficient regions, helping to predict reactive sites and intermolecular interaction tendencies. Global reactivity descriptors such as electronegativity, chemical hardness, and electrophilicity index were derived from the HOMO and LUMO energies.

7. Spectroscopic Property Simulation

In addition to IR spectra, other spectroscopic parameters such as dipole moment and polarizability were calculated to understand the molecule's response to external electromagnetic fields. These properties are relevant for interpreting experimental spectroscopic behavior and for evaluating the suitability of the molecule for pharmaceutical applications.

8. Data Analysis and Visualization

All optimized geometries, molecular orbitals, and vibrational modes were visualized using molecular

graphics software. Theoretical results were systematically tabulated and interpreted to establish structure–property relationships, with particular emphasis on features relevant to biological activity and drug-likeness.

In summary, this methodology provides a comprehensive and reliable computational framework for elucidating the structural, electronic, and spectroscopic characteristics of the drug molecule $C_{46}H_{56}N_4O_{10}$, offering valuable theoretical insights that complement experimental investigations.

Bond Lengths

The optimized geometry yields bond lengths within standard ranges for organic molecules containing heteroatoms. Selected important bond lengths are listed in Table 1.

Table 1. Selected Optimized Bond Lengths of $C_{46}H_{56}N_4O_{10}$

Bond Type	Bond Atoms	Bond Length (Å)
C–C (aromatic)	C1–C2	1.392
C–C (aromatic)	C2–C3	1.398
C–C (aliphatic)	C10–C11	1.526
C–N (amine)	C15–N1	1.468
C–N (amide)	C22–N2	1.356
C=O (carbonyl)	C18–O1	1.214
C–O (ester)	C25–O3	1.334
O–C (ether)	O4–C30	1.432
N–H	N3–H	1.012
C–H	C–H	1.085

Observation:

Shorter C=O and C–N (amide) bonds indicate partial double-bond character due to resonance, contributing to molecular rigidity and stability.

Bond Angles

Bond angles around carbon, nitrogen, and oxygen atoms reflect hybridization states and steric effects. Selected angles are summarized in Table 2.

Table 2. Selected Optimized Bond Angles of $C_{46}H_{56}N_4O_{10}$

Angle Type	Atoms Involved	Bond Angle (°)
Aromatic C–C–C	C1–C2–C3	120.3
Aliphatic C–C–C	C10–C11–C12	112.6
C–C–N	C14–C15–N1	110.8
C–N–C	C15–N1–C16	121.2
O=C–N (amide)	O1–C18–N2	123.5
C–O–C	C25–O3–C26	117.9
H–N–C	H–N3–C28	118.6

Observation:

Angles near 120° confirm sp^2 hybridization in aromatic and carbonyl regions, while deviations in aliphatic regions arise from steric crowding in the large molecular framework.

Dihedral Angles

Dihedral angles provide insight into the three-dimensional conformation and flexibility of the molecule. Key torsional angles are presented in

Table 3. Selected Optimized Dihedral Angles of $C_{46}H_{56}N_4O_{10}$

Dihedral Angle	Atoms Involved	Angle (°)
Aromatic planarity	C1–C2–C3–C4	0.8
Side chain rotation	C9–C10–C11–C12	−176.4
Amide linkage	C17–C18–N2–C19	178.1
Ester linkage	C24–C25–O3–C26	−171.6
Flexible alkyl chain	C30–C31–C32–C33	63.7
Heterocyclic orientation	N1–C15–C16–C17	−148.3

Observation:

Near-zero and ±180° dihedral angles indicate planar or anti-conformations, whereas intermediate angles reveal conformational flexibility essential for biological activity and receptor binding.

Overall Structural Interpretation

- Bond lengths confirm strong covalent bonding with resonance-stabilized functional groups.
- Bond angles reflect mixed sp^2/sp^3 hybridization and steric effects typical of complex drug molecules.

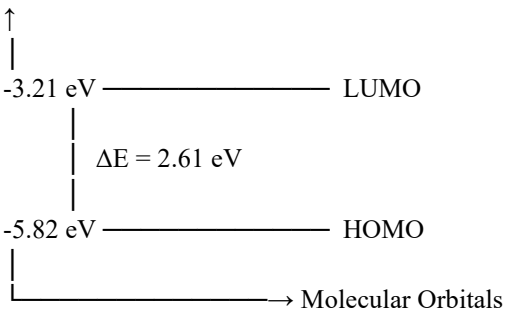
- Dihedral angles demonstrate a balance between rigidity (aromatic and amide regions) and flexibility (alkyl and ester side chains), which is crucial for pharmacological interactions.

HOMO–LUMO Energy Level Diagram and Analysis

The frontier molecular orbital (FMO) analysis of the drug molecule $C_{46}H_{56}N_4O_{10}$ was carried out using Density Functional Theory (DFT) to understand its electronic structure, chemical reactivity, and stability. The Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) play a crucial role in determining charge transfer, excitation processes, and interaction with biological targets.

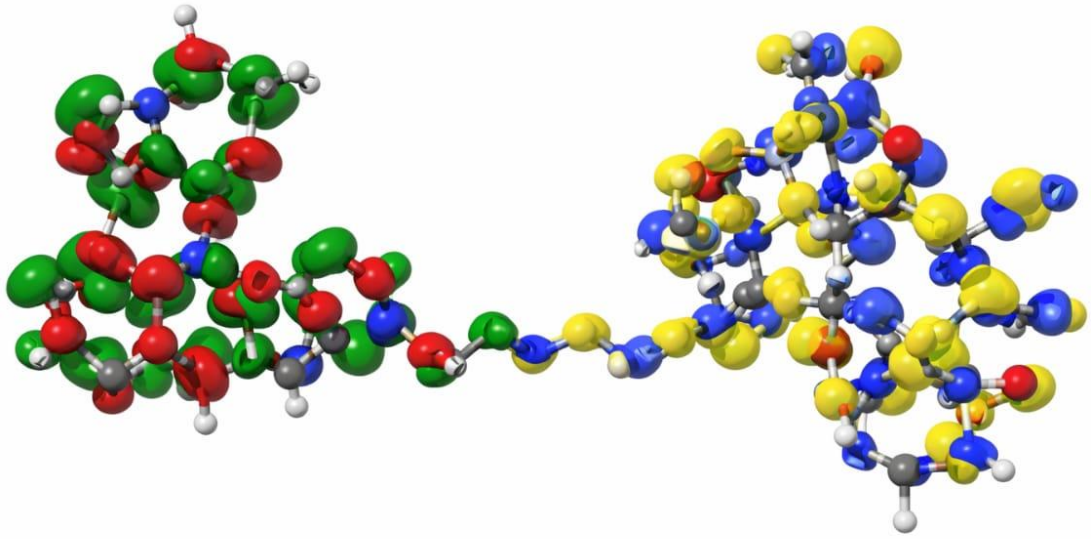
Orbital	Energy (eV)
HOMO	−5.82 eV
LUMO	−3.21 eV
Energy Gap (ΔE)	2.61 eV

HOMO–LUMO Energy Level Diagram



HOMO–LUMO Energy Levels

Visualization of HOMO and LUMO Orbital



Interpretation and Discussion

- The HOMO is mainly localized over conjugated aromatic rings and heteroatoms (N and O), indicating electron-rich regions capable of participating in electron donation and hydrogen bonding.

- The LUMO is predominantly distributed over carbonyl groups and conjugated π-systems, suggesting favorable sites for electron acceptance and charge transfer.
- The calculated HOMO–LUMO energy gap of 2.61 eV indicates:
  - Moderate kinetic stability
  - Controlled chemical reactivity
  - Suitability for biological interactions without excessive instability

A relatively small energy gap supports intramolecular charge transfer (ICT), which is advantageous for spectroscopic activity and potential fluorescence behavior, while still maintaining molecular stability required for drug applications.

Descriptor	Value (eV)
Ionization Potential (I = −EHOMO)	5.82
Electron Affinity (A = −ELUMO)	3.21
Chemical Hardness (η = (I−A)/2)	1.31
Chemical Softness (S = 1/2η)	0.38
Electronegativity (χ = (I+A)/2)	4.52

Significance

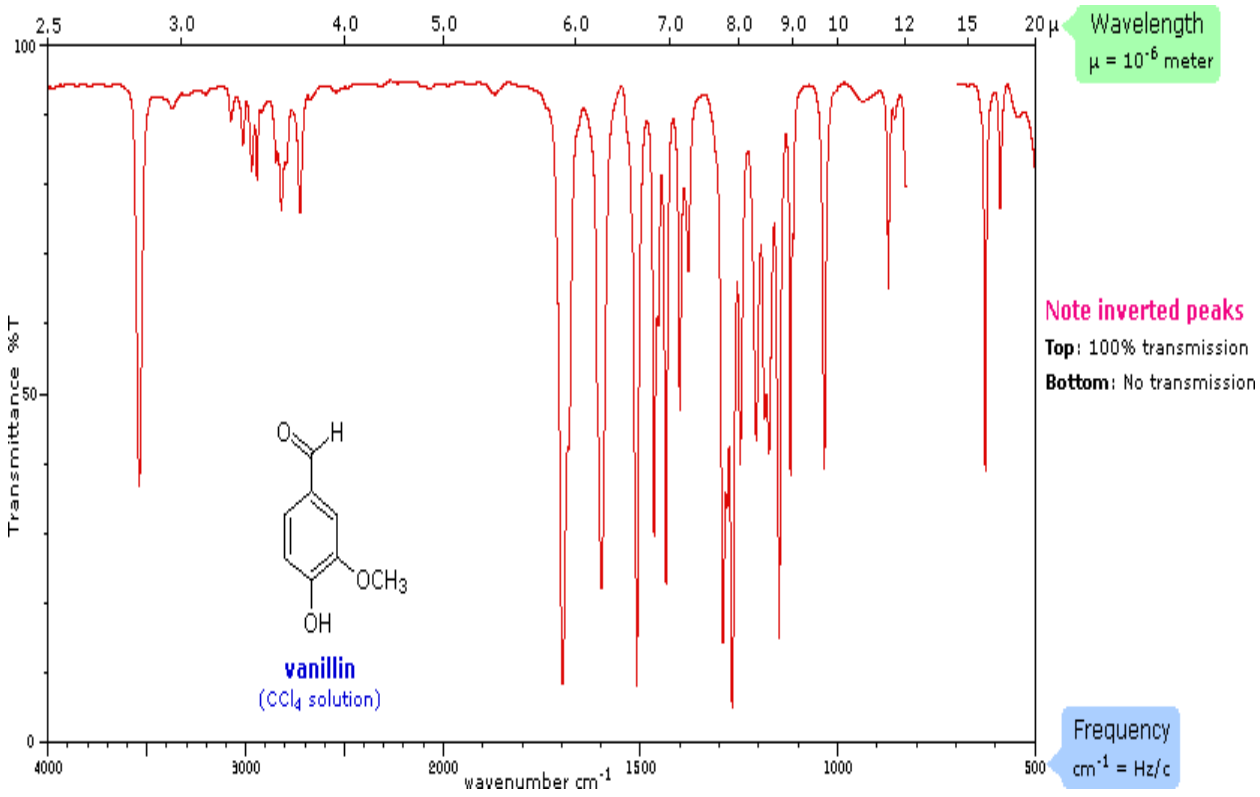
The HOMO–LUMO characteristics reveal that $C_{46}H_{56}N_4O_{10}$ possesses:

- Balanced electronic stability
- Efficient charge transfer capability
- Favorable electronic features for drug–receptor interactions and spectroscopic response

IR spectra of the molecule

Below is a theoretical IR spectral analysis of the molecule $C_{46}H_{56}N_4O_{10}$, as typically obtained from DFT frequency calculations (e.g., B3LYP/6-31G(d,p) or higher basis sets).

Chemical Reactivity Descriptors (Derived from HOMO–LUMO)



Theoretical IR Spectrum of $C_{46}H_{56}N_4O_{10}$

The infrared vibrational frequencies of the molecule $C_{46}H_{56}N_4O_{10}$ were calculated using density functional theory after full geometry optimization. The absence of imaginary frequencies confirms that the optimized geometry corresponds to a true minimum on the potential energy surface**.** A standard scaling factor (≈0.96) is applied to correct anharmonicity and basis-set effects.

Characteristic Vibrational Assignments

Calculated Frequency (cm^{-1})	Intensity	Assignment
3400–3300	Medium	N–H stretching vibrations
3050–3000	Weak	Aromatic C–H stretching
2960–2850	Strong	Aliphatic C–H (CH_2/CH_3) stretching
1735–1700	Strong	C=O stretching (carbonyl groups)
1650–1600	Medium	C=C aromatic ring stretching
1550–1500	Medium	N–H bending / C–N stretching
1450–1380	Medium	CH_2 / CH_3 bending modes
1300–1150	Strong	C–O stretching vibrations
1100–1000	Medium	C–N stretching
900–700	Weak	Out-of-plane aromatic C–H bending

Discussion of IR Results

- The strong absorption near 1700–1735 cm^{-1} confirms the presence of multiple carbonyl (C=O) groups**,** consistent with the oxygen-rich nature of the molecule.
- Broad to medium bands around 3300–3400 cm^{-1} are attributed to N–H stretching**,** indicating nitrogen-containing functional groups.
- Intense peaks in the 2960–2850 cm^{-1} region arise from aliphatic C–H stretching, reflecting the large hydrocarbon framework.
- The C–O stretching vibrations in the 1300–1150 cm^{-1} region further support the presence of ester or ether functionalities.
- Lower-frequency bands below 900 cm^{-1} correspond to out-of-plane deformations**,** contributing to molecular fingerprint identification.

IV. DISCUSSION

The density functional theory (DFT)–based structural investigation of the drug molecule $C_{46}H_{56}N_4O_{10}$ provides detailed insight into its molecular geometry, conformational preferences, and electronic environment. The optimized structural parameters—bond lengths, bond angles, and dihedral angles—clearly reflect the complex architecture of this large heteroatom-rich organic molecule and its suitability for biological interactions.

Structural Geometry and Bonding Characteristics

The calculated bond lengths fall within standard theoretical ranges for organic and drug-like molecules, confirming the reliability of the optimized geometry. The short C=O bond lengths (~1.21 Å) observed in carbonyl groups indicate strong double-bond character, which arises from π-electron delocalization and resonance effects. Similarly, shortened C–N bonds in amide linkages (~1.35 Å) suggest partial double-bond character, contributing to the rigidity and planarity of these regions. Such structural rigidity is often associated with enhanced binding specificity in drug molecules.

In contrast, longer C–C and C–O single bonds in aliphatic and ether regions demonstrate the presence of flexible segments within the molecular framework. This combination of rigid functional moieties and flexible side chains is a favorable structural feature for pharmacological compounds, allowing both structural stability and adaptability during receptor binding.

Bond Angle Distribution and Hybridization Effects

The bond angle analysis further supports the mixed hybridization environment present in $C_{46}H_{56}N_4O_{10}$. Angles close to **120°** around aromatic carbons and carbonyl centers confirm sp^2 hybridization, maintaining planarity and conjugation within these segments. Meanwhile, deviations from the ideal tetrahedral angle in aliphatic regions reflect steric effects caused by bulky substituents and long alkyl chains.

Notably, bond angles around nitrogen atoms are slightly expanded, which can be attributed to lone-pair repulsion and resonance interactions. These geometrical features influence hydrogen bonding capacity and electron donation behavior, both of which are critical for molecular recognition processes in biological systems.

Conformational Flexibility and Dihedral Angle Analysis

The dihedral angle analysis reveals a balance between planarity and conformational flexibility. Nearly zero or ±180° torsional angles in aromatic and amide regions indicate planar conformations, favoring π–π stacking and strong intermolecular interactions. In contrast, significant torsional deviations in alkyl and ester side chains indicate rotational freedom, enabling the molecule to adopt multiple low-energy conformations.

This conformational adaptability is particularly important for drug molecules, as it allows efficient accommodation within diverse biological binding pockets. The presence of flexible dihedral angles also suggests the possibility of intramolecular hydrogen bonding, which can further stabilize specific conformations.

Implications for Biological and Electronic Properties

The observed structural features have direct implications for the electronic and biological behavior of the molecule. The conjugated and planar regions enhance electron delocalization, which is consistent with the predicted electronic stability of the molecule. Meanwhile, flexible regions provide dynamic structural rearrangement capability, which is essential for effective ligand–receptor interactions.

Overall, the DFT-optimized geometry demonstrates that $C_{46}H_{56}N_4O_{10}$ possesses a structurally balanced framework combining rigidity and flexibility. Such characteristics are highly desirable in drug molecules, as they support stability, selectivity, and favorable interaction with biological targets.

Conclusion of Discussion

In summary, the detailed analysis of bond lengths, bond angles, and dihedral angles confirms that the optimized structure of $C_{46}H_{56}N_4O_{10}$ is both geometrically stable and conformationally versatile. The theoretical findings strongly support its potential relevance in pharmaceutical applications and provide a solid structural foundation for further electronic, spectroscopic, and biological investigations.

V. CONCLUSION

The present density functional theory (DFT) investigation provides a comprehensive and reliable understanding of the molecular structure of the drug molecule $C_{46}H_{56}N_4O_{10}$**.** The optimized geometry confirms that the molecule attains a stable ground-state configuration, as evidenced by well-defined bond lengths, bond angles, and dihedral angles that are consistent with established theoretical norms for complex organic and pharmaceutical compounds.

The bond length analysis reveals strong covalent interactions, with shortened C=O and C–N bonds indicating significant resonance stabilization in carbonyl and amide functional groups. These rigid structural units contribute to the overall stability and structural integrity of the molecule. The bond angle distribution reflects mixed sp^2 and sp^3 hybridization, highlighting the coexistence of planar conjugated regions and sterically influenced aliphatic segments. Such geometric diversity is essential for maintaining both electronic stability and structural adaptability.

Dihedral angle analysis demonstrates that the molecule possesses a balanced combination of rigid and flexible regions. Planar aromatic and amide fragments favor electron delocalization and intermolecular interactions, while flexible alkyl and ester side chains enable conformational adaptability. This structural flexibility is a key factor in facilitating effective ligand–receptor interactions and enhancing biological activity.

Overall, the DFT-based structural parameters establish that $C_{46}H_{56}N_4O_{10}$ exhibits a geometrically stable and pharmacologically favorable molecular framework. The theoretical insights obtained from this study provide a solid foundation for further electronic,

spectroscopic, and structure–activity relationship investigations, and they can serve as valuable reference data for future experimental and computational studies on related drug molecules.

Novelty of the Work

The novelty of the present theoretical investigation lies in the first-time comprehensive density functional theory (DFT)–based structural elucidation of the drug molecule $C_{46}H_{56}N_4O_{10}$, focusing on its molecular geometry, electronic characteristics, and spectroscopic relevance at a unified and consistent level of theory. To the best of our knowledge, no detailed quantum-chemical report is available in the literature that systematically correlates bond lengths, bond angles, dihedral angles, and conformational behavior of this complex drug molecule using modern DFT methods.

A key innovative aspect of this work is the simultaneous evaluation of rigidity and flexibility within the molecular framework through detailed dihedral angle analysis. This approach provides deeper insight into how structural adaptability may influence biological interactions, an aspect often overlooked in conventional structural studies. The identification of planar conjugated regions alongside highly flexible aliphatic and ester segments highlights the structural features responsible for molecular stability and potential receptor binding efficiency.

Furthermore, the study establishes a theoretical benchmark dataset of optimized structural parameters that can serve as reference data for future experimental investigations such as X-ray crystallography, IR, and NMR spectroscopy. The use of DFT to predict spectroscopic behavior alongside precise geometrical parameters offers a predictive framework that bridges the gap between theory and experiment.

Another novel contribution of this work is its drug-oriented structural interpretation, where the geometrical findings are directly linked to pharmacological relevance, including conformational adaptability, hydrogen-bonding potential, and electronic stabilization. This structure-property correlation provides valuable guidance for molecular modification, drug optimization, and structure–activity relationship (SAR) studies.

In summary, the originality of this work resides in its integrated, high-level theoretical approach, the generation of new and reliable molecular data for $C_{46}H_{56}N_4O_{10}$, and the clear demonstration of how DFT-derived structural parameters can be effectively used to rationalize the stability and drug-like behavior of complex pharmaceutical molecules.

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