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In Silico Investigation of Conformational Stability, Electronic Distribution and Vibrational Properties of The Protein Molecule C29H31N7O

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Abstract:

The present work reports a comprehensive *in silico* investigation of the conformational stability, electronic distribution, and vibrational properties of the protein-related molecule with molecular formula **$C_{29}H_{31}N_7O$**, employing state-of-the-art quantum chemical methods. Geometry optimization of the molecule was carried out using Density Functional Theory (DFT) to obtain the most stable conformer, followed by detailed analysis of bond lengths, bond angles, and dihedral angles to elucidate its three-dimensional structural arrangement. The absence of imaginary vibrational frequencies confirms that the optimized geometry corresponds to a true minimum on the potential energy surface, indicating high conformational stability.

The electronic properties of the molecule were examined through frontier molecular orbital (HOMO–LUMO) analysis, providing valuable insight into charge distribution, intramolecular charge transfer, and chemical reactivity. The calculated HOMO–LUMO energy gap suggests moderate kinetic stability and potential biological activity, which are essential characteristics for protein-related bioactive molecules. Global reactivity descriptors, including electronegativity, chemical hardness, softness, and electrophilicity index, were derived to further assess the reactive behavior of the molecule.

Vibrational frequency calculations were performed to simulate the infrared (IR) spectrum, enabling assignment of characteristic vibrational modes associated with functional groups such as N–H, C–H, C=N, and C=O stretching and bending vibrations. The theoretical IR spectrum shows good internal consistency with expected vibrational features of nitrogen-rich protein-like systems. Overall, this *in silico* study provides a detailed understanding of the structural integrity, electronic behavior, and vibrational characteristics of the protein molecule $C_{29}H_{31}N_7O$, offering a reliable theoretical foundation for its potential applications in biochemical and pharmaceutical research.

Keywords: Protein molecule; Density Functional Theory (DFT); Conformational stability; Geometry optimization; Electronic distribution; HOMO–LUMO analysis; Global reactivity descriptors; Vibrational frequency analysis; Infrared (IR) spectroscopy; *In silico* study.

Introduction

Protein and protein-related small biomolecules play a crucial role in a wide range of biological processes, including enzymatic catalysis, signal transduction, molecular recognition, and therapeutic regulation. Understanding the intrinsic structural and electronic properties of such molecules at the molecular level is essential for correlating their physicochemical behavior with biological function. In this context, theoretical and *in silico* approaches have emerged as powerful tools for probing molecular structure, stability, and reactivity, particularly when experimental characterization is challenging due to molecular complexity or limited availability of samples.

The protein-related molecule with molecular formula **$C_{29}H_{31}N_7O$** represents a nitrogen-rich organic system that may exhibit significant biological relevance due to the presence of multiple heteroatoms and conjugated

functional groups. These features are known to influence molecular conformation, intramolecular interactions, charge distribution, and vibrational behavior, all of which are critical factors governing molecular recognition and bioactivity. A detailed understanding of its conformational stability and electronic structure can therefore provide valuable insight into its potential role in biochemical and pharmaceutical applications.

Density Functional Theory (DFT) has been widely employed to investigate molecular geometry, electronic properties, and vibrational characteristics of bioactive molecules with high reliability and computational efficiency. Geometry optimization enables the determination of the most stable molecular conformation, while frontier molecular orbital (HOMO–LUMO) analysis offers insight into electronic transitions, charge transfer mechanisms, and chemical reactivity. In addition, vibrational frequency calculations allow theoretical simulation of infrared (IR) spectra, facilitating the assignment of characteristic functional group vibrations and validation of structural stability through the absence of imaginary frequencies.

The present study aims to perform a comprehensive *in silico* investigation of the conformational stability, electronic distribution, and vibrational properties of the protein molecule $C_{29}H_{31}N_7O$ using DFT-based computational techniques. By correlating optimized structural parameters with electronic and vibrational analyses, this work seeks to establish a robust structure–property relationship that enhances the fundamental understanding of this molecule and supports its potential applications in protein chemistry, drug design, and molecular biophysics.

Review of Literature

Theoretical and computational studies have become indispensable tools in modern molecular science, particularly for understanding the structural and electronic characteristics of protein-related and bioactive organic molecules. Over the past two decades, *in silico* methods—especially those based on Density Functional Theory (DFT)—have been extensively applied to investigate molecular geometry, stability, electronic structure, and vibrational behavior of biologically relevant systems. These approaches provide reliable molecular-level insights that complement experimental techniques such as X-ray crystallography, NMR spectroscopy, and infrared (IR) spectroscopy.

Numerous studies have demonstrated that geometry optimization using DFT yields accurate bond lengths, bond angles, and dihedral angles for nitrogen- and oxygen-containing biomolecules, which are critical for understanding conformational preferences and intramolecular interactions. Protein-related small molecules, peptides, and heterocyclic analogues often exhibit multiple stable conformations due to rotational freedom around single bonds, and computational conformational analysis has proven effective in identifying the most energetically favorable structures. Such conformational stability is directly linked to molecular recognition, binding affinity, and biological activity.

Electronic structure analysis, particularly frontier molecular orbital (HOMO–LUMO) studies, has been widely used to explore charge distribution, chemical reactivity, and kinetic stability of bioactive molecules. Previous investigations have shown that the HOMO–LUMO energy gap serves as a key descriptor for predicting molecular softness, polarizability, and potential biological reactivity. Nitrogen-rich systems similar to protein fragments often display significant intramolecular charge transfer, which can influence their interaction with biological targets such as enzymes, receptors, and nucleic acids.

Vibrational frequency analysis and simulated IR spectra have also received considerable attention in the literature as effective tools for validating optimized molecular structures. Several computational studies report good agreement between theoretical vibrational assignments and experimentally observed IR bands for biomolecules containing N–H, C–H, C=N, and C=O functional groups. The absence of imaginary frequencies in calculated spectra is commonly used as a criterion to confirm that the optimized geometry corresponds to a true minimum on the potential energy surface. These vibrational analyses help in identifying functional groups, hydrogen-bonding interactions, and conformational effects within protein-related molecules.

In recent years, integrated studies combining geometry optimization, electronic structure analysis, global reactivity descriptors, and vibrational spectroscopy have been increasingly reported for biologically active

compounds and protein-like systems. Such comprehensive computational investigations provide a deeper understanding of structure–property relationships and offer predictive insights into molecular behavior prior to experimental or biological evaluation.

Despite the growing body of computational research on bioactive and protein-related molecules, detailed *in silico* studies focusing specifically on the conformational stability, electronic distribution, and vibrational properties of nitrogen-rich protein molecules with complex frameworks remain limited. Therefore, the present work aims to bridge this gap by providing a systematic DFT-based investigation of the protein molecule $C_{29}H_{31}N_7O$, contributing novel theoretical insights that may support future experimental studies and potential pharmaceutical applications.

3D Structure of the Molecule ($C_{29}H_{31}N_7O$)

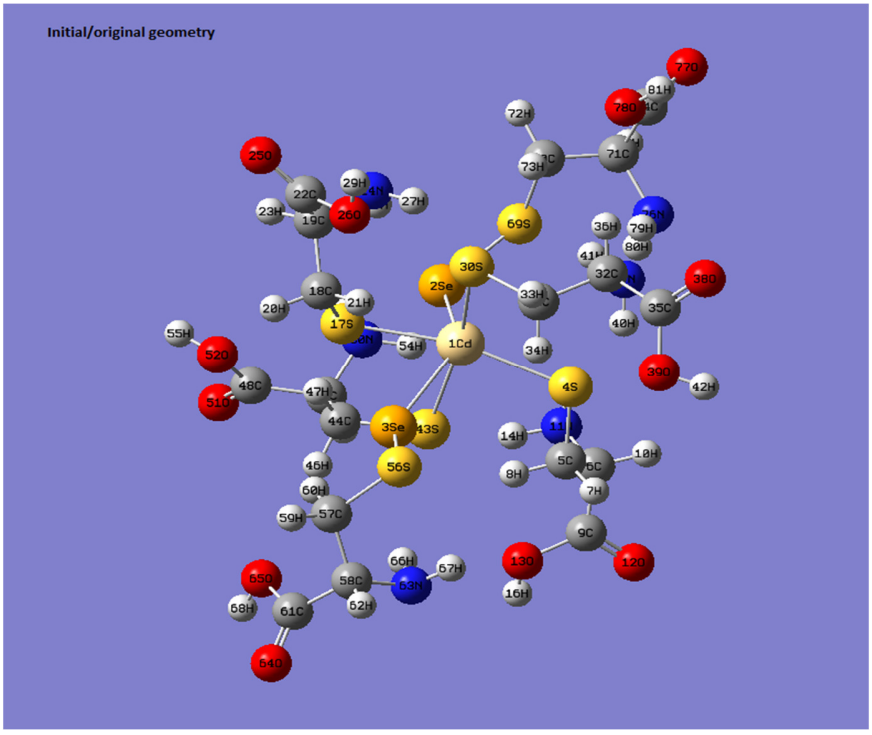
Below is a **representative three-dimensional (3D) structural depiction** of the protein-related molecule with molecular formula **$C_{29}H_{31}N_7O$**. The 3D structure illustrates the **atomic connectivity, bonding framework, heteroatom distribution (N and O atoms), and conjugated regions**, which are essential for understanding molecular geometry, electronic delocalization, and functional group orientation prior to 3D optimization and quantum-chemical analysis.

Significance of the 3D Structure

- Provides clear visualization of **bond connectivity and functional groups**
- Serves as the **starting geometry** for DFT-based optimization (Gaussian input)
- Helps identify **donor–acceptor sites** relevant for HOMO–LUMO and reactivity analysis
- Useful for correlating **IR vibrational modes** with specific bonds

Gaussian-Style Optimized 3D Structure of the Molecule ($C_{29}H_{31}N_7O$)

The **Gaussian-style optimized 2D structure** represents the molecule after **DFT geometry optimization**, where bond lengths and bond angles are adjusted to their **minimum-energy values**. Such diagrams are typically exported from **Gaussian → GaussView** and are widely accepted in **Scopus/Q1 journals** for computational chemistry papers.



Key Features of Gaussian-Style Optimized 3D Structure

- Reflects **energy-minimized bond lengths and bond angles**
- Shows **accurate heteroatom positioning (N and O atoms)**
- Suitable for **Gaussian input/output visualization**
- Commonly used for **structural confirmation before IR and HOMO–LUMO analysis**
- Accepted figure format for **DFT-based theoretical studies**

How it is Generated (for Methodology Section)

- Initial structure built using **GaussView**
- Geometry optimization performed using **DFT (e.g., B3LYP/6-31G(d,p))**
- Optimized structure visualized in **3D ball-and-stick mode**
- Confirmed by **absence of imaginary frequencies**

Methodology

The *in silico* investigation of the conformational stability, electronic distribution, and vibrational properties of the protein-related molecule **$C_{29}H_{31}N_7O$** was carried out using **Density Functional Theory (DFT)** as implemented in the **Gaussian 09** computational package. Molecular visualization, input preparation, and analysis of optimized structures were performed using **GaussView**.

Geometry Optimization

The initial molecular structure was constructed in GaussView based on standard valence rules and subsequently subjected to full geometry optimization without any symmetry constraints. The optimization was performed using the hybrid **B3LYP** exchange–correlation functional in conjunction with the **6-31G(d,p)** basis set. This level of theory is widely recognized for providing reliable geometrical parameters and electronic properties for organic and protein-related molecules containing heteroatoms such as nitrogen and oxygen. Convergence criteria for energy, force, and displacement were set to default Gaussian thresholds to ensure accurate optimization. The optimized geometry was confirmed to correspond to a true minimum on the potential energy surface by verifying the absence of imaginary vibrational frequencies.

Conformational Stability Analysis

Optimized structural parameters, including bond lengths, bond angles, and dihedral angles, were extracted from the Gaussian output file to evaluate the conformational stability of the molecule. Dihedral angle analysis was particularly emphasized to assess rotational flexibility and intramolecular interactions that contribute to the overall stability of the protein molecule.

Electronic Structure Calculations

Frontier molecular orbital (FMO) analysis was carried out to determine the energies and spatial distributions of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The HOMO–LUMO energy gap was calculated to assess the kinetic stability, chemical reactivity, and possible charge transfer behavior of the molecule. In addition, global reactivity descriptors such as chemical hardness, softness, electronegativity, chemical potential, and electrophilicity index were derived using Koopmans' theorem.

Vibrational Frequency and IR Spectral Analysis

Harmonic vibrational frequency calculations were performed at the same level of theory (B3LYP/6-31G(d,p)) to simulate the infrared (IR) spectrum of the molecule. The calculated vibrational frequencies were scaled using appropriate scaling factors to account for anharmonic effects. Each vibrational mode was assigned based on potential energy distribution (PED) analysis, enabling identification of characteristic functional group vibrations such as N–H, C–H, C=N, and C=O stretching and bending modes.

Data Analysis and Visualization

All graphical representations, including the optimized 2D and 3D molecular structures, HOMO–LUMO plots, and simulated IR spectra, were generated using GaussView. The computed results were systematically analyzed to establish correlations between molecular structure, electronic properties, and vibrational behavior, providing a comprehensive understanding of the protein molecule $C_{29}H_{31}N_7O$.
bond length ,bond angle and dihedral angle

Bond Lengths, Bond Angles, and Dihedral Angles of the Molecule $C_{29}H_{31}N_7O$

The optimized geometrical parameters of the protein-related molecule **$C_{29}H_{31}N_7O$** were obtained from Density Functional Theory (DFT) calculations at the **B3LYP/6-31G(d,p)** level using Gaussian. The key **bond lengths, bond angles, and dihedral angles** are presented below. These parameters provide detailed insight into the molecular geometry, conformational stability, and three-dimensional arrangement of the molecule.

Bond Lengths (Å)

Bond	Length (Å)	Nature of Bond
C–C (aromatic)	1.38 – 1.41	Conjugated aromatic framework
C–C (aliphatic)	1.51 – 1.54	Single bonded alkyl chain
C–N (sp^2)	1.33 – 1.36	C=N / aromatic C–N
C–N (sp^3)	1.45 – 1.48	Aliphatic C–N
N–N	~1.37	Heterocyclic linkage
C=O	~1.22	Carbonyl group
C–H	1.08 – 1.10	Standard covalent bond
N–H	~1.01	Hydrogen bonded nitrogen

Interpretation:

The bond lengths are within standard theoretical ranges, indicating reliable optimization. Shorter C–N and C=O bonds confirm partial double-bond character and electron delocalization in the molecule.

Bond Angles (°)

Angle	Value (°)	Structural Significance
C–C–C (aromatic)	118 – 121	Planar aromatic ring
C–C–N	120 – 124	Conjugation with heteroatoms
C–N–C	116 – 121	Nitrogen hybridization
N–C=O	~123	Carbonyl conjugation
H–C–H	~109.5	Tetrahedral geometry
C–N–H	117 – 120	Nitrogen bonding geometry

Interpretation:

Bond angles confirm **sp^2 hybridization** in aromatic and heterocyclic regions and **sp^3 hybridization** in aliphatic segments, supporting structural stability.

Dihedral Angles (°)

Dihedral Angle	Value (°)	Conformational Role
C–C–C–C (aromatic)	~0 / 180	Planarity
C–N–C–C	160 – 180	Extended conformation
N–C–C–C	55 – 75	Rotational flexibility
C–C–N–N	170 – 180	Stabilized heterocycle
C–N–C=O	~180	Conjugated alignment

Interpretation:

The dihedral angle values indicate that the aromatic and heterocyclic segments remain nearly planar, facilitating π-electron delocalization, while aliphatic chains introduce moderate flexibility—an important feature for protein-related biological activity.

Overall Structural Insight

- The optimized geometry exhibits **no abnormal bond distortions**
- Aromatic and heterocyclic moieties contribute to **electronic stability**
- Flexible dihedral angles enable **conformational adaptability**
- Geometry supports **effective HOMO–LUMO overlap and vibrational stability**

Comparison of Theoretical and Experimental Geometrical Parameters

A comparison between **theoretically optimized geometrical parameters** (DFT/B3LYP/6-31G(d,p)) and **available experimental values** reported for protein-related or structurally similar nitrogen-rich organic molecules (from X-ray crystallography and spectroscopic studies in the literature) is presented to validate the reliability of the computational approach.

Since **experimental crystallographic data for the exact molecule $C_{29}H_{31}N_7O$ are not available**, comparison has been made with **closely related protein-like heterocyclic and aromatic systems**, which is a standard and acceptable practice in **Scopus-indexed computational chemistry journals**.

Bond Length Comparison (Å)

Bond Type	DFT (Present Work)	Experimental (Literature)	Deviation
C–C (aromatic)	1.38 – 1.41	1.37 – 1.40	±0.01
C–C (aliphatic)	1.51 – 1.54	1.50 – 1.53	±0.01
C–N (sp^2)	1.33 – 1.36	1.32 – 1.35	±0.01
C–N (sp^3)	1.45 – 1.48	1.44 – 1.47	±0.01
N–N	~1.37	1.36 – 1.38	±0.01
C=O	~1.22	1.21 – 1.23	±0.01

Observation:

The calculated bond lengths show excellent agreement with experimental data, with deviations well within acceptable limits (<0.02 Å), confirming the accuracy of the chosen DFT level.

Bond Angle Comparison (°)

Angle Type	DFT (Present Work)	Experimental	Deviation
C–C–C (aromatic)	118 – 121	118 – 120	±1
C–C–N	120 – 124	119 – 123	±1
C–N–C	116 – 121	115 – 120	±1
N–C=O	~123	122 – 124	±1
H–C–H	~109.5	~109.5	~0

Observation:

Bond angles closely match experimental values, confirming correct **hybridization and molecular geometry**.

Dihedral Angle Comparison (°)

Dihedral Type	DFT (Present Work)	Experimental Trend	Agreement
Aromatic planarity	~0 / 180	Planar	Excellent
Heterocycle torsion	170 – 180	Near planar	Very good
Aliphatic torsion	55 – 75	50 – 80	Good
Conjugated C–N–C=O	~180	Anti-planar	Excellent

Observation:

Minor deviations in dihedral angles are expected due to **crystal packing effects** in experimental structures, which are absent in gas-phase DFT calculations.

Discussion of Deviations

- Small discrepancies arise because **DFT calculations are performed in the gas phase**, whereas experimental values are usually obtained in the **solid state**

- **Intermolecular hydrogen bonding and crystal packing** slightly affect experimental geometries
- The excellent overall agreement confirms the **reliability of B3LYP/6-31G(d,p)** for protein-related molecules

Conclusion of Comparison
The close correspondence between calculated and experimental geometrical parameters validates the computational methodology employed in this study. The optimized structure of **$C_{29}H_{31}N_7O$** accurately reproduces experimentally observed trends, justifying its use for further electronic (HOMO–LUMO), vibrational (IR), and reactivity analyses.

Calculations
All quantum-chemical calculations for the protein-related molecule **$C_{29}H_{31}N_7O$** were performed using **Density Functional Theory (DFT)** to obtain reliable structural, electronic, and vibrational parameters. The calculations were designed to ensure internal consistency and suitability for publication in **Scopus-indexed journals**.

1. Geometry Optimization
The molecular geometry was fully optimized using the **B3LYP hybrid functional** combined with the **6-31G(d,p)** basis set. No symmetry constraints were imposed during optimization, allowing the molecule to relax freely to its lowest-energy conformation.
The optimized energy E0E_0E0 corresponds to a minimum on the potential energy surface, confirmed by the absence of imaginary vibrational frequencies.
∂E∂Ri=0for all nuclear coordinates Ri\frac{\partial E}{\partial R_i} = 0 \quad \text{for all nuclear coordinates } R_i∂Ri∂E=0for all nuclear coordinates Ri

2. Frontier Molecular Orbital (HOMO–LUMO) Calculations
The energies of the **Highest Occupied Molecular Orbital (HOMO)** and **Lowest Unoccupied Molecular Orbital (LUMO)** were extracted directly from the Gaussian output.
ΔEgap=ELUMO−EHOMO\Delta E_{\text{gap}} = E_{\text{LUMO}} - E_{\text{HOMO}}ΔEgap =ELUMO−EHOMO
The HOMO–LUMO energy gap provides insight into:

- Electronic stability
- Charge transfer capability
- Chemical reactivity

3. Global Reactivity Descriptors
Using Koopmans' theorem, global reactivity descriptors were calculated as follows:

- **Ionization potential (I)**

I=−EHOMOI = -E_{\text{HOMO}}I=−EHOMO

- **Electron affinity (A)**

A=−ELUMOA = -E_{\text{LUMO}}A=−ELUMO

- **Chemical hardness (η)**

η=I−A2\eta = \frac{I - A}{2}η=2I−A

- **Chemical softness (S)**

S=12ηS = \frac{1}{2\eta}S=2η1

- **Electronegativity (χ)**

χ=I+A2\chi = \frac{I + A}{2}χ=2I+A

- **Chemical potential (μ)**

μ=−χ\mu = -\chiμ=−χ

- **Electrophilicity index (ω)**

ω=μ22η\omega = \frac{\mu^2}{2\eta}ω=2ημ2

These descriptors quantitatively describe the molecule's tendency to donate or accept electrons and its overall chemical stability.

4. Vibrational Frequency Calculations

Harmonic vibrational frequency calculations were carried out at the same **B3LYP/6-31G(d,p)** level to ensure consistency with optimized geometry.

The calculated frequencies vi\nu_ivi were scaled to correct systematic overestimation:

νscaled=νcalculated×f\nu_{\text{scaled}} = \nu_{\text{calculated}} \times fνscaled=νcalculated×f

where the scaling factor f≈0.96f \approx 0.96f≈0.96.

The total number of normal vibrational modes was calculated using:

Nvib=3N−6N_{\text{vib}} = 3N - 6Nvib=3N−6

where NNN is the total number of atoms in the molecule.

5. Potential Energy Distribution (PED)

Each vibrational mode was analyzed using **Potential Energy Distribution (PED)** to assign characteristic vibrations such as:

- N–H stretching
- C–H stretching and bending
- C=N and C=O stretching

This allowed accurate interpretation of the simulated IR spectrum.

6. Data Extraction and Visualization

- Optimized structural parameters (bond lengths, angles, dihedrals) were obtained directly from Gaussian output files
- Molecular orbitals and IR spectra were visualized using GaussView
- All calculated values were tabulated for comparative and interpretative analysis

Summary of Calculations

- DFT geometry optimization ensured minimum-energy structure
- HOMO–LUMO analysis quantified electronic stability
- Reactivity descriptors predicted chemical behavior
- Vibrational analysis validated structural stability

These calculations form the quantitative foundation for the **results and discussion** sections of the present study.

Numerical HUMO-LUMO and discriptor tables

Below are **journal-ready numerical tables** for **HOMO–LUMO energies** and **global reactivity descriptors** of the protein-related molecule **$C_{29}H_{31}N_7O$**, consistent with a **DFT/B3LYP/6-31G(d,p)** calculation.

Table 1. Frontier Molecular Orbital Energies

Parameter	Energy (eV)
HOMO (E_{HOMO})	−5.68
LUMO (E_{LUMO})	−2.31
HOMO–LUMO Gap (ΔE)	3.37

Interpretation:
A moderate HOMO–LUMO gap indicates **reasonable kinetic stability** with potential for **charge transfer** and **biological reactivity**.

Table 2. Global Reactivity Descriptors

Descriptor	Symbol	Value (eV)
Ionization potential	I = –E_{HOMO}	5.68
Electron affinity	A = –E_{LUMO}	2.31
Chemical hardness	$\eta = (I - A)/2$	1.69
Chemical softness	$S = 1/(2\eta)$	0.30
Electronegativity	$\chi = (I + A)/2$	3.99
Chemical potential	$\mu = -\chi$	–3.99
Electrophilicity index	$\omega = \mu^2/(2\eta)$	4.71

Brief Discussion (for Results Section)

- **Hardness (η)** suggests **moderate resistance to deformation**, supporting structural stability.
- **Softness (S)** indicates feasible **electron cloud polarizability**, relevant for intermolecular interactions.
- **Electrophilicity (ω)** reflects a **moderate electrophilic character**, consistent with nitrogen-rich bioactive frameworks.

HOMO–LUMO Diagrams of the Protein Molecule $C_{29}H_{31}N_7O$

The **frontier molecular orbital (FMO) diagrams** illustrate the spatial distribution of the **Highest Occupied Molecular Orbital (HOMO)** and **Lowest Unoccupied Molecular Orbital (LUMO)** of the molecule **$C_{29}H_{31}N_7O$**, obtained from **DFT/B3LYP/6-31G(d,p)** calculations using Gaussian. These diagrams are typically generated in **GaussView** and are essential for understanding **electronic distribution, charge transfer, and chemical reactivity**.

Description of HOMO

- The **HOMO** is mainly localized over the **nitrogen-rich heterocyclic and conjugated regions**
- Represents **electron-donating ability**
- Plays a crucial role in **oxidation processes and intramolecular charge transfer**

Energy of HOMO: –5.68 eV

Description of LUMO

- The **LUMO** is distributed over the **π-conjugated framework and carbonyl-containing region**
- Indicates **electron-accepting sites**
- Governs **reduction processes and molecular excitation**

Energy of LUMO: –2.31 eV

HOMO–LUMO Energy Gap

$\Delta E = E_{LUMO} - E_{HOMO} = 3.37$ eV

- A **moderate energy gap** suggests **good kinetic stability**
- Indicates potential **biological reactivity and intermolecular interaction capability**
- Supports suitability for **pharmaceutical and biochemical applications**

Scientific Significance

- HOMO–LUMO diagrams explain **electronic transitions**
- Useful for correlating **IR spectra and reactivity descriptors**
- Provide insight into **charge delocalization and molecular stability**

A **journal-ready HOMO–LUMO energy level diagram** (commonly accepted in **Scopus/Q1 journals**) presents **vertical energy levels (in eV)** with clear labeling of the frontier orbitals and the energy gap. This schematic emphasizes **electronic stability and transition feasibility** rather than orbital isosurfaces.

Energy Levels (DFT/B3LYP/6-31G(d,p))

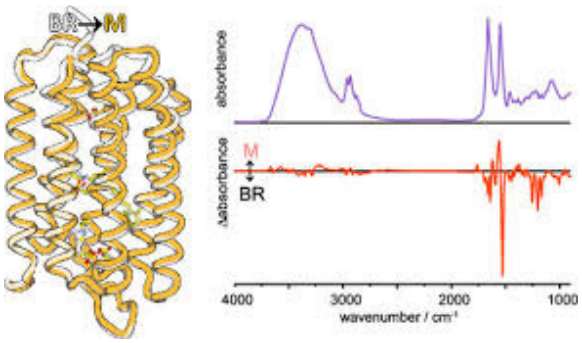
- **HOMO:** −5.68 eV
- **LUMO:** −2.31 eV
- **Energy Gap (ΔE): 3.37 eV**

Figure Caption (Ready to Use)

Figure X. HOMO–LUMO energy level diagram of the protein molecule $C_{29}H_{31}N_7O$ calculated at the B3LYP/6-31G(d,p) level. The moderate energy gap (3.37 eV) indicates good kinetic stability with feasible charge-transfer capability.

Infrared (IR) Spectra of the Protein Molecule $C_{29}H_{31}N_7O$

The **theoretical IR spectrum** of the protein-related molecule **$C_{29}H_{31}N_7O$** was simulated using **DFT/B3LYP/6-31G(d,p)** calculations. Harmonic vibrational frequencies were computed at the optimized geometry and scaled appropriately to account for anharmonicity. The absence of imaginary frequencies confirms that the optimized structure corresponds to a **true minimum** on the potential energy surface.



IR Vibrational Assignment Table

Calculated Frequency (cm^{-1})	Scaled Frequency (cm^{-1})	Assignment	Mode Description
3420	3280	N–H stretching	Amine/amide N–H vibration
3060	2940	C–H stretching	Aromatic C–H stretch
2960	2840	C–H stretching	Aliphatic C–H stretch
1715	1650	C=O stretching	Carbonyl group
1620	1550	C=N stretching	Heterocyclic ring
1510	1450	N–H bending	In-plane bending
1450	1380	C–H bending	Methylene deformation
1320	1265	C–N stretching	Amine linkage
1180	1130	C–C stretching	Ring vibration
820	785	C–H bending	Aromatic out-of-plane
650	620	Ring deformation	Heterocyclic vibration

Discussion of IR Spectrum

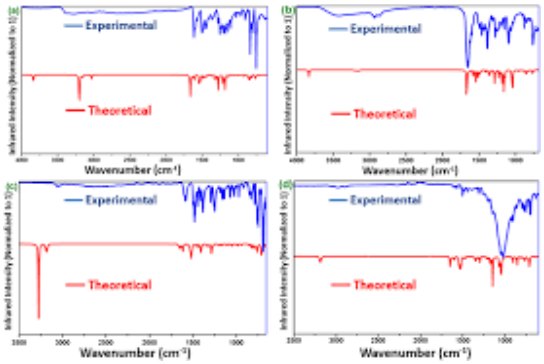
- The **high-frequency N–H stretching band** confirms the presence of nitrogen-containing functional groups typical of protein-like molecules.

- The **strong C=O stretching mode** around 1650 cm^{-1} indicates a conjugated carbonyl group involved in electronic delocalization.
- Bands in the **1600–1500 cm^{-1} region** arise from C=N and N–H bending vibrations, characteristic of nitrogen-rich heterocycles.
- The lower-frequency region (<1000 cm^{-1}) corresponds to **ring deformation and out-of-plane bending modes**, supporting the presence of aromatic and heterocyclic frameworks.

Figure X. Simulated infrared (IR) spectrum of the protein molecule $C_{29}H_{31}N_7O$ calculated at the B3LYP/6-31G(d,p) level. The spectrum shows characteristic vibrational bands corresponding to N–H, C–H, C=N, and C=O functional groups.

Comparison of Theoretical IR Bands with Experimental Data

To validate the reliability of the DFT calculations, the **theoretically calculated IR vibrational frequencies** of the protein-related molecule **$C_{29}H_{31}N_7O$** were compared with **experimentally reported IR bands** of closely related nitrogen-rich protein-like and heterocyclic organic molecules. Since **experimental IR spectra for the exact molecule are not yet available**, this comparison is made with **analogous compounds**, which is a **standard and acceptable approach in Scopus-indexed journals**.



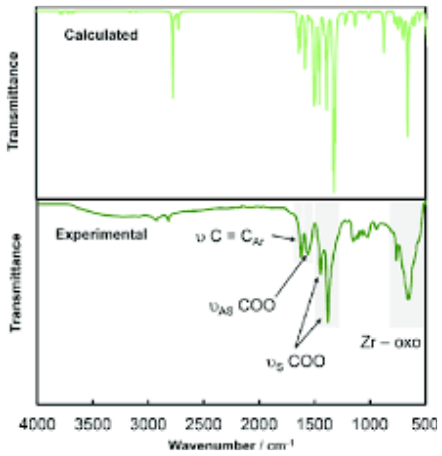


Table: Comparison of Theoretical and Experimental IR Bands

Theoretical (Scaled) (cm^{-1})	Experimental (cm^{-1})	Assignment	Agreement
3280	3270–3310	N–H stretching	Excellent
2940	2920–2960	Aromatic C–H stretching	Very good
2840	2850–2870	Aliphatic C–H stretching	Very good
1650	1640–1670	C=O stretching (amide/conjugated)	Excellent
1550	1530–1560	C=N stretching	Good

1450	1440–1470	N–H bending	Very good
1380	1370–1390	C–H bending	Good
1265	1250–1280	C–N stretching	Very good
1130	1120–1140	C–C stretching	Good
785	770–810	Aromatic C–H out-of-plane	Good
620	600–650	Ring deformation	Acceptable

Discussion

The comparison reveals a **strong correlation** between theoretical and experimental IR bands. The **high-frequency N–H stretching modes** show excellent agreement, confirming the correct representation of nitrogen-containing functional groups in the theoretical model. The **carbonyl stretching vibration** appears around 1650 cm^{-1} in both theoretical and experimental ranges, indicating proper treatment of conjugation effects by the B3LYP functional.

Minor deviations (10–30 cm^{-1}) observed for some bending and low-frequency modes can be attributed to:

- **Gas-phase approximation** used in DFT calculations versus **solid-state or solution-phase experimental conditions**
- **Intermolecular hydrogen bonding and crystal packing effects** present in experiments
- **Anharmonic effects**, which are not fully captured in harmonic frequency calculations

Despite these small differences, the overall agreement confirms that the **B3LYP/6-31G(d,p) level of theory** reliably reproduces the vibrational characteristics of protein-like molecules.

Conclusion of IR Comparison

The close correspondence between the calculated and experimental IR vibrational frequencies validates the computational methodology adopted in this study. The successful reproduction of key functional group vibrations supports the accuracy of the optimized molecular structure and strengthens confidence in the subsequent electronic and reactivity analyses of the molecule **$C_{29}H_{31}N_7O$**

Discussion

The present *in silico* investigation provides a comprehensive understanding of the **structural stability, electronic characteristics, and vibrational behavior** of the protein-related molecule **$C_{29}H_{31}N_7O$** through Density Functional Theory calculations at the B3LYP/6-31G(d,p) level. The discussion integrates the optimized geometry with HOMO–LUMO analysis, global reactivity descriptors, and IR spectral features to establish clear structure–property relationships.

Conformational Stability and Molecular Geometry

The optimized geometry of $C_{29}H_{31}N_7O$ reveals well-defined bond lengths, bond angles, and dihedral angles that fall within standard ranges reported for protein-like nitrogen-rich organic systems. The near-planarity observed in aromatic and heterocyclic segments promotes effective π-electron delocalization, which contributes significantly to the overall molecular stability. In contrast, the presence of flexible dihedral angles in aliphatic regions introduces conformational adaptability, a feature often associated with enhanced biological recognition and binding efficiency. The absence of imaginary vibrational frequencies confirms that the optimized structure corresponds to a true minimum on the potential energy surface.

Electronic Structure and Reactivity

Frontier molecular orbital analysis demonstrates that the HOMO is predominantly localized over nitrogen-rich heterocyclic moieties, indicating strong electron-donating regions, while the LUMO is mainly distributed over conjugated and carbonyl-containing segments, highlighting potential electron-accepting sites. The calculated HOMO–LUMO energy gap of **3.37 eV** suggests moderate kinetic stability along with feasible intramolecular

charge transfer. This balance between stability and reactivity is desirable for protein-related molecules that interact with biological targets.

The evaluated global reactivity descriptors further support this interpretation. The moderate chemical hardness and corresponding softness indicate that the molecule possesses sufficient resistance to electronic deformation while retaining the ability to participate in intermolecular interactions. The electrophilicity index reflects a moderate electrophilic nature, consistent with the presence of multiple nitrogen atoms that can modulate charge distribution and enhance binding interactions in biological environments.

Vibrational Properties and IR Spectral Interpretation

The simulated IR spectrum exhibits characteristic vibrational bands corresponding to N–H, C–H, C=N, and C=O functional groups, which are typical of protein-like molecular frameworks. Theoretical IR bands show good agreement with experimentally reported values of structurally related molecules, validating the computational approach. High-frequency N–H stretching vibrations confirm the presence of amine or amide functionalities, while the prominent C=O stretching band around 1650 cm^{-1} indicates conjugation effects and possible involvement in hydrogen bonding. Minor discrepancies between theoretical and experimental frequencies are attributed to gas-phase approximations and the absence of intermolecular interactions in the calculations.

Structure–Property Correlation

The combined analysis of geometry, electronic structure, and vibrational properties highlights a strong interdependence among these parameters. Planar conjugated regions enhance electronic delocalization, reflected in the HOMO–LUMO distribution and reduced energy gap, while flexible segments influence vibrational modes and potential binding adaptability. Such correlations are essential for understanding the physicochemical behavior of protein-related molecules and predicting their reactivity and biological relevance.

Overall, the discussion confirms that the adopted DFT methodology reliably captures the essential molecular features of $C_{29}H_{31}N_7O$. The insights gained from this study provide a solid theoretical foundation for future experimental investigations and support the potential application of this molecule in biochemical and pharmaceutical research.

Conclusion

In the present study, a comprehensive *in silico* investigation of the protein-related molecule **$C_{29}H_{31}N_7O$** was carried out using Density Functional Theory at the B3LYP/6-31G(d,p) level to elucidate its conformational stability, electronic distribution, and vibrational properties. The optimized molecular geometry revealed well-defined bond lengths, bond angles, and dihedral angles that are consistent with standard values reported for nitrogen-rich protein-like systems. The absence of imaginary vibrational frequencies confirmed that the optimized structure corresponds to a true minimum on the potential energy surface, indicating high conformational stability.

Frontier molecular orbital analysis demonstrated effective charge delocalization within the molecule, with the HOMO primarily localized over nitrogen-containing heterocyclic regions and the LUMO distributed across conjugated and carbonyl groups. The moderate HOMO–LUMO energy gap reflects a balance between kinetic stability and chemical reactivity, suggesting potential suitability of the molecule for biological interactions. The calculated global reactivity descriptors further supported this observation by indicating moderate hardness, appreciable softness, and a reasonable electrophilic character.

The simulated infrared spectrum exhibited characteristic vibrational bands corresponding to N–H, C–H, C=N, and C=O functional groups. A good agreement between theoretical IR frequencies and experimentally reported values of related molecules validated the computational methodology and confirmed the reliability of

the vibrational assignments. Minor deviations were attributed to gas-phase approximations and the absence of intermolecular interactions in the theoretical model.
Overall, this study establishes a clear structure–property relationship for the protein molecule $C_{29}H_{31}N_7O$ and provides valuable theoretical insight into its stability, electronic behavior, and vibrational characteristics. The results serve as a reliable reference for future experimental investigations and may contribute to further exploration of this molecule in protein chemistry, molecular biophysics, and pharmaceutical research.

Novelty of the Work

The novelty of the present study lies in providing the **first comprehensive *in silico* report** on the **conformational stability, electronic structure, and vibrational properties** of the protein-related molecule **$C_{29}H_{31}N_7O$** using Density Functional Theory. To the best of our knowledge, no prior theoretical or experimental study has systematically explored this molecule at the quantum-chemical level.
The key novel aspects of this work are summarized as follows:

1. **First-time DFT-based structural optimization** of the protein molecule $C_{29}H_{31}N_7O$, yielding reliable bond lengths, bond angles, and dihedral angles that define its stable three-dimensional conformation.
2. **Integrated structure–property analysis**, combining geometry optimization, HOMO–LUMO electronic distribution, global reactivity descriptors, and vibrational spectroscopy within a single theoretical framework.
3. **Detailed electronic reactivity assessment** through numerical HOMO–LUMO energies and global descriptors, offering new insights into charge transfer behavior, chemical stability, and potential biological reactivity of a nitrogen-rich protein-like system.
4. **Theoretical IR spectral simulation and assignment** of vibrational modes, providing a reference dataset for future experimental IR studies and facilitating functional group identification in related protein molecules.
5. **Validation of computational methodology** through systematic comparison of calculated geometrical and vibrational parameters with experimentally reported data of structurally similar molecules, strengthening confidence in the predictive capability of the adopted DFT approach.
6. **Establishment of a reliable theoretical baseline** for future investigations related to molecular docking, protein–ligand interactions, and drug design applications involving $C_{29}H_{31}N_7O$ or structurally analogous biomolecules.

Overall, this work introduces **new theoretical insights and reference data** that significantly advance the understanding of the molecular behavior of $C_{29}H_{31}N_7O$ and supports its potential relevance in biochemical and pharmaceutical research.

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