Journal homepage: www.scienceletters.researchfloor.org

Contents list available at Journal of e-Science Letters

Journal of e-Science Letters

Proceeding Original Article | ISSN :3041-5454

Density Functional Theory Study of the Structural, Electronic and Reactivity Properties of 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide (A1)

Santosh R Mannopantar[1], Jitendra R. Jahagirdar[2], Ramesh D[3], Mangesh S. Jadhav[4], and Dayanand Lalasangi*[5]

[1]*Department of Physics, GFGC, Kalaghatagi, Dharwad, Karnataka, India*
[2]*Department of Physics, Sri. K. H. Patil GFGC, Hulakoti, Gadag, Karnataka, India*
[3]*Department of Chemistry, GFGC, Shikaripura, Shivamogga, Karnataka, India*
[4]*Department of Physics, JSS Arts, Science and Commerce College, Gokak, Belagavi, Karnataka, India*
[5]*Department of Physics, GFGC, Kengeri, Bengaluru, Karnataka, India*

ABSTRACT

A comprehensive quantum chemical investigation was carried out on 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide (A1) to evaluate its structural, electronic, and molecular reactivity characteristics. Density Functional Theory (DFT) calculations were performed using the B3LYP functional with the 6-31G(d,p) basis set in Gaussian 09. The optimized geometry was validated by frequency analysis, confirming the absence of imaginary vibrational modes. Frontier molecular orbital analysis demonstrated effective intramolecular π-electron delocalization, with the HOMO mainly localized over the donor region and the LUMO distributed across the acceptor fragment, indicating pronounced charge-transfer behavior. The calculated HOMO–LUMO energy gap of 4.2758 eV suggests favorable kinetic stability and moderate chemical reactivity. Molecular electrostatic potential mapping revealed electron-rich regions around the carbonyl oxygen and thiocarbonyl sulfur atoms, identifying the principal reactive sites of the molecule. Furthermore, quantum chemical descriptors confirmed its balanced electron-donating and electron-accepting ability. These findings establish A1 as a structurally stable donor–acceptor system with promising potential for optoelectronic, nonlinear optical, and molecular sensing applications.

Keywords: *Density Functional Theory; B3LYP; 6-31G(d,p); Naphthofuran; HOMO–LUMO; Molecular electrostatic potential.*

Introduction

The design and investigation of π-conjugated organic molecules containing heteroaromatic and donor–acceptor structural motifs have received considerable attention because of their distinctive electronic, optical, and molecular recognition properties[1], [2], [3].

Citation: Santosh R Mannopantar, Jitendra R. Jahagirdar, Ramesh D, Mangesh S. Jadhav, and Dayanand Lalasangi (2025). Density Functional Theory Study of the Structural, Electronic and Reactivity Properties of 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide (A1).
Journal of e-Science Letters.
DOI: https://doi.org/10.51470/eSL.2025.6.4.119

Received: 25 September 2025
Revised: 29 October 2025
Accepted: 30 November 2025
Available: December 28 2025

Corresponding Authors: **Dayanand Lalasangi**
Email: **dayanandlalasangi@gmail.com**

Extended π-electron delocalization can facilitate intramolecular charge transfer (ICT), thereby influencing molecular polarity, frontier orbital distribution, chemical reactivity, and optical response[4], [5]. Such characteristics are particularly important in the development of functional organic materials for applications in optoelectronics, nonlinear optics, molecular sensing, and related electronic devices. The incorporation of fused heteroaromatic systems into conjugated molecular architectures provides an effective strategy for modifying their electronic structure and charge-transfer characteristics [4], [6], [7], [8].

Naphthofuran derivatives constitute an interesting class of fused heterocyclic compounds because the extended aromatic framework provides a conjugated pathway for electron delocalization. In particular, halogen substituents such as bromine and chlorine can influence molecular polarization and the distribution of electron density within a conjugated framework. Understanding the relationship between these structural features and the resulting electronic properties is therefore important for assessing the potential functionality of such compounds[9], [10].

The present study focuses on 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide (A1), a molecule containing a brominated naphthofuran moiety connected through a carbonyl hydrazinecarbothioamide bridge to a chlorophenyl group.

The presence of oxygen, nitrogen, sulfur, bromine, and chlorine atoms is also expected to contribute to the molecular electrostatic distribution and to influence the preferred sites for intermolecular interactions.

Density Functional Theory (DFT) has become an important computational approach for obtaining molecular geometries and evaluating electronic properties of molecular systems [11], [12], [13], [14], [15]. Hybrid exchange–correlation functionals such as B3LYP combine Hartree–Fock exchange with density-functional correlation contributions and have been extensively employed for molecular structure and electronic-property calculations. The B3LYP functional is constructed from the Becke three-parameter exchange formulation together with the Lee–Yang–Parr correlation functional.

Frontier molecular orbital (FMO) analysis provides useful information concerning the electron-donating and electron-accepting characteristics of a molecule. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), together with their energy difference, can provide qualitative information about molecular stability, electronic excitation, charge-transfer characteristics, and chemical reactivity [13], [16], [17]. In addition, global reactivity descriptors such as ionization potential, electron affinity, electronegativity, chemical potential, chemical hardness, softness, and electrophilicity can provide complementary information concerning the tendency of a molecular system to donate or accept electron density.

Molecular electrostatic potential (MEP) and electrostatic potential (ESP) analyses provide a spatial description of the molecular charge distribution and are particularly useful for identifying electron-rich and electron-deficient regions on a molecular surface. Such information can assist in locating potential sites for electrophilic and nucleophilic interactions and in understanding possible intermolecular interactions [14], [18], [19].

Donor–acceptor (D–A) π-conjugated heterocyclic compounds have attracted considerable attention because of their remarkable optical, electronic, and charge-transfer properties, making them promising candidates for organic light-emitting diodes, nonlinear optical (NLO) materials, fluorescent sensors, and photovoltaic devices[20], [21]. The incorporation of fused aromatic heterocycles together with electron-withdrawing substituents enhances π-electron delocalization and facilitates efficient intramolecular charge transfer (ICT), which governs the photo physical behaviour of these molecules [2], [13], [16], [22], [23].

In the present work, 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide was investigated as a novel donor–π–acceptor molecular system. The optimized geometry was verified through harmonic vibrational frequency analysis, followed by evaluation of the thermodynamic parameters, HOMO and LUMO energies, HOMO–LUMO energy gap, and global chemical reactivity descriptors[24], [25], [26]. The molecular framework comprises a brominated naphthofuran moiety linked through a carbonyl hydrazinecarbothioamide bridge to a 3-chlorophenyl group, producing an extended conjugated architecture with significant electron delocalization. The presence of bromine, chlorine, oxygen, nitrogen, and sulfur atoms is expected to influence the electronic distribution, molecular polarity, and intermolecular interactions, thereby enhancing its optical and electronic performance.

To obtain a detailed understanding of the molecular electronic structure, Density Functional Theory (DFT) calculations were carried out using the B3LYP hybrid exchange–correlation functional with the 6-31G (d, p) (d, p) basis set. The optimized molecular geometry was employed to evaluate the frontier molecular orbitals (HOMO–LUMO), energy gap, molecular electrostatic potential (MEP), and global reactivity descriptors. The combined structural and theoretical study provides valuable insight into the relationship between the molecular architecture and its electronic and optical properties, highlighting the potential of 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide as a promising functional material for optoelectronic and sensing applications.

Computational Details:

All quantum chemical calculations were performed using the Gaussian 09 software package. The molecular geometry of the synthesized brominated pyridine–thioamide hydrazone derivative was fully optimized using Density Functional Theory (DFT) with the Becke three-parameter Lee–Yang–Parr (B3LYP) hybrid exchange–correlation functional and the 6-31G (d, p)(d,p) basis set [13], [14], [15]. No symmetry constraints were imposed during geometry optimization.

To verify that the optimized structure corresponded to a true minimum on the potential energy surface, harmonic vibrational frequency calculations were carried out at the same B3LYP/6-31G (d, p) (d,p) level, and no imaginary frequencies were observed [27], [27], [28]. The optimized geometry was subsequently used for the calculation of frontier molecular orbital energies (HOMO and LUMO), HOMO–LUMO energy gap, molecular electrostatic potential (MEP), and global reactivity parameters. Molecular orbital and MEP surface visualizations were generated using Gauss view 5.0.

Results and Discussion

Various computational studies of the substituted 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide (A1) molecule were carried out. These computational studies of structural, charge distribution, thermodynamical concepts, spectroscopic absorption and emission studies, quantum chemical analysis, ESP, and MEP are presented.

Structure and geometric properties:

The molecular structure of the molecule 2-[(8-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide was built using GaussView 5.0 and was fully optimized using the Gaussian 09 program package with the Opt + Freq calculation method for geometry optimization. In addition, calculations were made using the DFT/B3LYP/6-31G (d, p) method. The geometry optimization procedure was carried out by introducing initial coordinates consistent with standard chemical values and searching for equilibrium geometry. Frequencies were calculated to determine whether the optimized geometry is a minimum on the potential energy surface. Figure.1 shows the optimized molecular structure for A1. In order to study the effects of electron excitation on the molecular geometry of A1, calculations using B3LYP/6 31G(d,p) for ground states, were carried out.

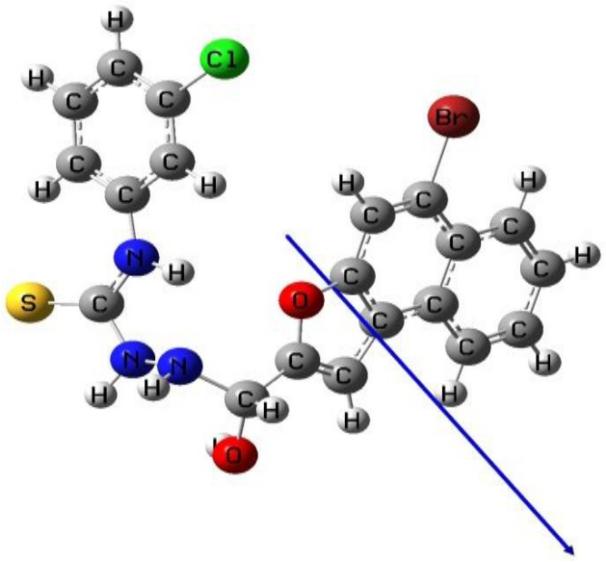

Figure.1: Optimized molecular structure of A1

The thermodynamic properties of A1 theoretically calculated at the level of theory DFT/B3LYP/6-31G (d, p) are collected in Table.1. They can be used to estimate the energetic contribution of translation, rotation, and vibration, as well as the enthalpy, entropy, and other thermodynamic properties of the optimized molecule. The translational and rotational energies of the molecule are equal to 0.889 kcal mol $^{-1}$ and contribute only a small part to the total energy of A1. The main source of thermal energy is the vibrational one, which amounted to 213.036 kcal mol $^{-1}$. The total amount of thermal energy of A1 is 214.813 kcal mol^{-1}, and it is predominantly determined by the vibrational energy component. Nuclear repulsion energy is 3135.602 Hartree and is related to the optimized geometry of A1. The zero-point vibrational energy (ZPVE) is 199.758 kcal mol^{-1}, and it is the minimum vibrational energy of the molecule. According to calculations, the entropy of A1 is 174.864 cal mol^{-1} K^{-1}. It is determined by the number of translational, rotational, and vibrational degrees of freedom of the molecule. For A1, the rotational constants A, B, and C are 0.13896 GHz, 0.09880 GHz, and 0.06619 GHz, respectively. This difference indicates the asymmetry of the molecule, which also follows from the geometry optimization. The rotational temperature is also lowest for A1: for the axis, and for axes and, the rotational temperatures were found to be equal to 0.00667 K, 0.00474 K, and 0.00318 K, respectively. Thus, the thermodynamic properties of A1 calculated at the level of theory DFT/B3LYP/6-31G (d, p) show the stability of the optimized geometry and good thermodynamic behavior. Such behavior is primarily determined by the high vibrational energy, which is the dominant component of the total energy of the molecule.

Table 1: Calculated thermodynamic parameters of A1 with DFT theory using B3LYP/6-31G (d, p) basis set

Parameters	DFT/B3LYP/6-31G (d, p)
Energy [kcal mol^{-1}]	
Translational	0.889
Rotational	0.889
Vibrational	213.036
Total	214.813
Nuclear repulsion energy [Hartree's]	3135.602
Zero-point vibrational energy [kcal mol^{-1}]	199.758
Entropy S [cal mol^{-1} K^{-1}]	174.864
Rotational constants [GHz]	
A	0.13896
B	0.09880
C	0.06619
Rotational temperatures [Kelvin]	
A	0.00667
B	0.00474
C	0.00318

Frontier molecular orbitals and quantum chemical calculations:

Frontier molecular orbital (FMO) analysis offers valuable information about a molecule's electronic structure, charge-transfer mechanism, and reactivity. The energies and shapes of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) determine the nature of the electron donor and acceptor regions. The energy of the HOMO is related to the ionization potential of the molecule, while the energy of the LUMO is connected to the electron affinity. Therefore, the interaction between HOMO and LUMO is an essential factor in charge transfer processes, which determines the reactivity and stability of the molecule.

The three-dimensional distribution of frontier molecular orbitals (FMOs) of A1 is presented in **Figure.2**, based on the B3LYP/6-31G (d, p) (d, p) calculation method. It can be seen that the HOMO is dominated by π bonding, while the LUMO is characterized by π anti-bonding. Therefore, the major contribution to the electronic transition of the molecule is π→π transition. Apart from that, the distribution of FMOs reveals electron transfer within the molecule, which helps identify the mechanism of action. In molecular orbital diagrams, the red color represents the negative lobe, while the blue color stands for the positive lobe.

The energy gap between the HOMO and LUMO orbitals was found to be 4.2758 eV. The significant value of ΔE indicates that A1 has a good kinetic stability and moderate chemical reactivity. On the other hand, the calculated value of ΔE proves efficient electron communication in the molecule, which supports the optical properties of A1 and its potential application in optoelectronic and molecular electronic devices. Additionally, the considerable HOMO-LUMO gap (4.2758 eV) implies that A1 has moderate reactivity and sufficient kinetic stability, while the reduced possibility of intramolecular charge recombination makes it attractive for organic optoelectronic applications.

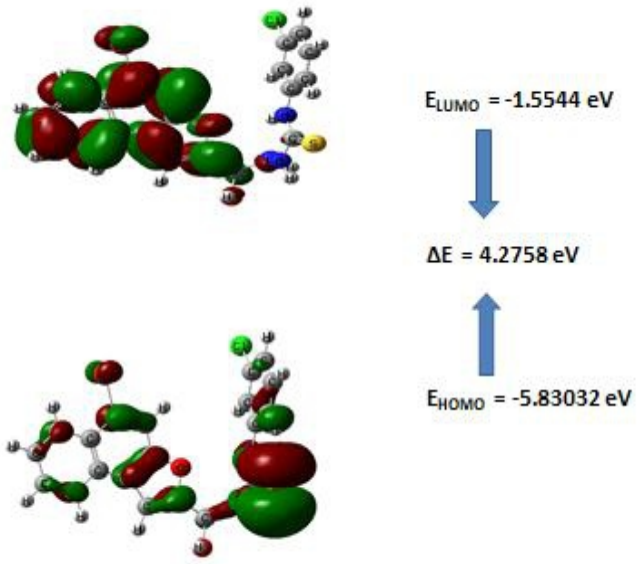

Figure.2: Representation of frontier molecular orbitals of A1 in vacuum medium using DFT method

From Koopmans' theorem, it can be inferred that the ionization potential (I) and electron affinity (A) can be determined using the frontier molecular orbital energies. This is because I = − E HOMO and A = − E LUMO. Thus, ionization potential and electron affinity energies give information about the charge-transfer ability, electronic structure, and reactivity of the molecule.

The calculated HOMO and LUMO energies are further used to compute other quantum chemical descriptors, namely, the HOMO–LUMO energy gap (Eg), chemical hardness (η), chemical potential (μ), chemical softness (S), electronegativity (χ), and global electrophilicity index (ω). The quantum chemical properties of A1 in gas phase and solvents are presented in Table.6. The descriptors are mostly used to predict molecular stability, electron donation and acceptance potentials, and chemical reactivity of the compound. From Table.2, the energy gap is relatively high, which implies that A1 molecule has good kinetic stability and low chemical reactivity. In addition, the global electrophilicity index of A1 is 3.18 eV, which means the molecule can accept electron density effectively. Hence, A1 has good electronic stability and can be potentially used in optoelectronics and related devices.

Table 2: Quantum chemical properties of A1 with vacuum

Molecules	E_{HOMO} eV	E_{LUMO}eV	Ionization Potential I eV	Electron affinity A eV	Electronegativity χ eV	Chemical hardness η eV	Chemical potential μ eV	Chemical softness S eV	Electrophilici index ω eV
A1	-5.830	-1.554	5.8303	1.5544	3.6923	2.1379	-3.692	0.2338	3.1885

Electrostatic potential:

Electrostatic potential (ESP) analysis is an effective tool for investigating the electronic characteristics and intermolecular interactions of a molecule. It provides a visual representation of the charge distribution on the molecular surface and enables the identification of regions susceptible to electrophilic and nucleophilic attack. Consequently, ESP mapping is widely employed to predict the reactive sites and interaction behavior of molecular systems.

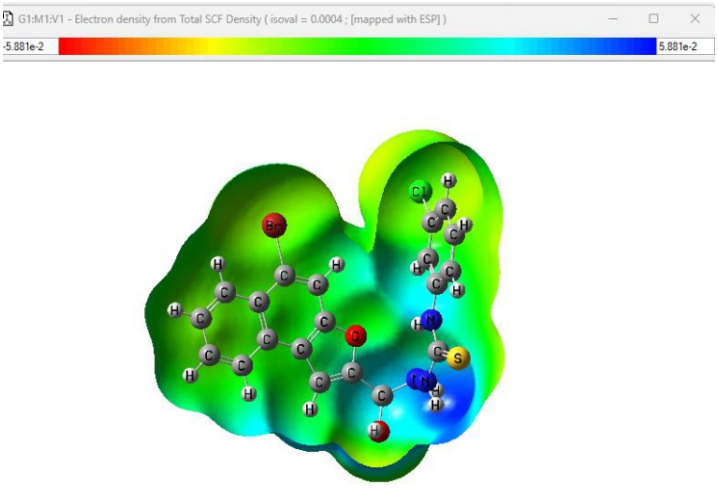

Fig.3: ESP mapping of A1 in Vacuum

The calculated ESP distribution of A1 in the gas phase is illustrated in Figure.3. The electrostatic potential values are distributed within the range of −0.05881 eV to +0.05881 eV. Regions exhibiting negative electrostatic potential correspond to electron-rich areas that are more favorable for electrophilic attack, whereas regions with positive electrostatic potential represent electron-deficient sites that are more susceptible to nucleophilic attack. The ESP surface therefore provides valuable insight into the charge distribution, molecular reactivity, and potential intermolecular interactions of A1, supporting its structural and electronic characterization.

Conclusion

The DFT study of 2-[(5-bromonaphtho[2,1-b]furan-2-yl)carbonyl]-N-(3-chlorophenyl)hydrazinecarbothioamide (A1) at the B3LYP/6-31G(d,p) level confirms a stable optimized molecular structure. The HOMO–LUMO analysis indicates π→π* charge-transfer characteristics with an energy gap of 4.2758 eV, suggesting good kinetic stability and moderate chemical reactivity. The calculated global reactivity descriptors and electrostatic potential distribution further provide insight into its electron-donating/accepting properties and reactive sites.

Overall, A1 exhibits favorable electronic characteristics, indicating potential for further investigation in optoelectronic, nonlinear-optical, and molecular-sensing applications.

Acknowledgements

I would like to express my sincere gratitude to the Commissioner, Department of Collegiate Education, Government of Karnataka, for the valuable support and encouragement extended towards the completion of this research article. I am deeply thankful for the opportunities and institutional support provided, which have contributed significantly to the successful completion of this research work.

Conference Note

This article was accepted for publication in the conference proceedings of the 8th World Congress on Materials Science and Engineering, held on March 27–28, 2025 (8th Edition) at SRH Berlin | University of Applied Sciences, Germany, organized by Mind Authors.

References

1. D. Lalasangi, S. M. Hanagodimath, T. Khanadal, B. Padmashali, and M. S. Jadhav, "Solvent Effects on the Absorption and Emission Spectra of the 5-amino-1-bromoindolizin-3-ylmethanone Molecule," *J. Fluoresc.*, 2024, doi: 10.1007/s10895-024-03732-7.
2. J. Thipperudrappa, U. P. Raghavendra, and M. Basanagouda, "Photophysical characteristics of biologically active 4-aryloxymethyl coumarins 4PTMBC and 1IPMBC," *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, vol. 136, no. PC, pp. 1475–1483, 2015, doi: 10.1016/j.saa.2014.10.039.
3. M. S. Mehata, A. K. Singh, and R. K. Sinha, "Investigation of charge-separation/change in dipole moment of 7-azaindole: Quantitative measurement using solvatochromic shifts and computational approaches," *J. Mol. Liq.*, vol. 231, no. February, pp. 39–44, 2017, doi: 10.1016/j.molliq.2017.01.091.
4. A. Atif, B. Ahmed, H. A. Sir, S. Mohammed, and Z. Abdellah, "Current Chemistry Letters," *Curr. Chem. Lett.*, vol. 15, pp. 101–116, 2026, doi: 10.5267/j.ccl.2025.10.006.
5. R. Alphonse, A. Varghese, L. George, and A. Nizam, "Estimation of ground state and excited state dipole moments of a novel Schiff base derivative containing 1, 2, 4-triazole nucleus by solvatochromic method," *J. Mol. Liq.*, vol. 215, pp. 387–395, 2016, doi: 10.1016/j.molliq.2015.12.050.
6. Y. Nefedov, N. Darmograi, M. Obushak, and V. Matiychuk, "O (S)," *Curr. Chem. Lett.*, vol. 14, pp. 723–732, 2025, doi: 10.5267/j.ccl.2025.9.001.
7. Y. Nechesnyi, S. Kemskyi, A. Grozav, N. Yakovychuk, K. Yutilova, and M. Vovk, "Current Chemistry Letters," *Curr. Chem. Lett.*, vol. 15, pp. 1–16, 2026, doi: 10.5267/j.ccl.2025.12.001.

8. R. V. Shingalapur, K. M. Hosamani, R. S. Keri, and M. H. Hugar, "Derivatives of benzimidazole pharmacophore: Synthesis, anticonvulsant, antidiabetic and DNA cleavage studies," *Eur. J. Med. Chem.*, vol. 45, no. 5, pp. 1753–1759, 2010, doi: 10.1016/j.ejmech.2010.01.007.
9. A. Kmita and A. Roczniak, "Implementation of nanoparticles in materials applied in foundry engineering," *Arch. Foundry Eng.*, vol. 17, no. 3, pp. 205–209, 2017, doi: 10.1515/afe-2017-0116.
10. M. S. Hameed, J. J. Princice, and N. R. Babu, "Effect of silver doping on optical properties of nanoflower *ZnO* thin films prepared by spray pyrolysis technique," *J. Mater. Sci. Mater. Electron.*, vol. 0, no. 0, p. 0, 2017, doi: 10.1007/s10854-017-6592-4.
11. A. S. Pirzada et al., "Physicochemical properties , pharmacokinetic studies , DFT approach , and antioxidant activity of nitro and chloro indolinone derivatives," *Front. Chem.*, no. March, pp. 1–15, 2024, doi: 10.3389/fchem.2024.1360719.
12. M. Ghosh and S. Sinha, "Solvatochromic Stokes shift and determination of excited state dipole moments of free base and zinc octaethylporphyrin," *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, vol. 150, no. June, pp. 959–965, 2015, doi: 10.1016/j.saa.2015.06.057.
13. Y. Sun, X. Liang, Y. Zhao, and J. Fan, "Solvent effects on the absorption and fluorescence spectra of rhaponticin: Experimental and theoretical studies," *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, vol. 102, pp. 194–199, 2013, doi: 10.1016/j.saa.2012.10.013.
14. Y. Gülseven Sidir and I. Sidir, "Solvent effect on the absorption and fluorescence spectra of 7-acetoxy-6-(2,3-dibromopropyl)-4,8-dimethylcoumarin: Determination of ground and excited state dipole moments," *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, vol. 102, pp. 286–296, 2013, doi: 10.1016/j.saa.2012.10.018.
15. M. A. Gabal, S. A. K. Elroby, and A. Y. Obaid, "Synthesis and characterization of nano-sized ceria powder via oxalate decomposition route," *Powder Technol.*, vol. 229, pp. 112–118, 2012, doi: 10.1016/j.powtec.2012.06.017.
16. Y. Sun, X. Liang, Y. Zhao, and J. Fan, "Solvent effects on the absorption and fluorescence spectra of rhaponticin: Experimental and theoretical studies," *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, vol. 102, no. July 2017, pp. 194–199, 2013, doi: 10.1016/j.saa.2012.10.013.
17. C. Polymers, "Electrical and Electrochemical Properties of Conducting Polymers," *Polymers*, 2017, doi: 10.3390/polym9040150.
18. S. Patil et al., "Investigation of Biogenic Silver nanoparticles Concentrations Impact on Novel Benzofuran Derivative and Their Electrochemical Study," *Bionanoscience*, vol. 13, no. 2, pp. 744–759, 2023, doi: 10.1007/s12668-023-01092-3.
19. S. More, O. Patil, S. Chillargikar, D. Lalasangi, and S. M. Hanagodimath, "DFT-Based Quantum Chemical Analysis of Coumarin Derivatives," *J. Fluoresc.*, vol. 1, no. 1, pp. 37–46, 2025.
20. D. Mathew, S. Sasidharan, P. Saudagar, S. Sujatha, and P. Parameswaran, "meso-Carbazole decorated BODIPYs – an electron donor–acceptor system with excellent fluorosolvato/vapochromic behavior, aggregation-induced emission, and antileishmanial activity," *New J. Chem.*, pp. 8277–8290, 2023, doi: 10.1039/d3nj00747b.
21. S. A. Hussain, "An Introduction to Fluorescence Resonance Energy Transfer (FRET)," *arXiv Prepr. arXiv0908.1815*, 2009, doi: 10.7237/sjp/268.
22. M. Pietrzak, M. Józefowicz, A. Bajorek, and J. R. Heldt, "Experimental and Theoretical Studies of the Spectroscopic Properties of Chalcone Derivatives," *J. Fluoresc.*, vol. 27, no. 2, pp. 537–549, 2017, doi: 10.1007/s10895-016-1981-2.
23. M. Khadem Sadigh, M. S. Zakerhamidi, S. M. Seyed Ahmadian, M. Johari-Ahar, and L. Zare Haghighi, "Environment and solute-solvent interaction effects on photo-physical behaviors of Folic acid and Folinic acid drugs," *J. Mol. Struct.*, vol. 1125, no. August, pp. 177–185, 2016, doi: 10.1016/j.molstruc.2016.06.068.
24. T. Boutadghart, K. Zaki, Y. Merroun, A. Sbai, and R. Ghailane, "Current Chemistry Letters," *Curr. Chem. Lett.*, vol. 15, pp. 17–34, 2026, doi: 10.5267/j.ccl.2025.11.004.
25. R. Kumari, A. Varghese, L. George, and Y. N. Sudhakar, "Effect of solvent polarity on the photophysical properties of chalcone derivatives," *RSC Adv.*, vol. 7, no. 39, pp. 24204–24214, 2017, doi: 10.1039/c7ra01705g.
26. A. L. R. S.Vidhya, "Ournal of," *Asian J. Chem.*, vol. 29, no. 8, pp. 1757–1760, 2017.
27. J. Coates, "Interpretation of Infrared Spectra , A Practical Approach Interpretation of Infrared Spectra , A Practical Approach," *Encycl. Anal. Chem.*, pp. 10815–10837, 2000, doi: DOI: 10.1002/9780470027318.
28. C. A. Royer, "Fluorescence spectroscopy.," *Methods Mol. Biol.*, vol. 40, pp. 65–89, 1995, doi: 10.1385/0-89603-301-5:65.