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Exploring solvent effects on reactivity, NLO properties, and toxicological interactions of 2'-((4,6-dimethoxy-1,3,5-triazin-2-yl)carbonyl)-1,1,6'-trifluoro-N-methylmethanesulfonamide

L. Sasikala^a, M. Prabhakaran^a  , P. Rajesh^b, G. Jayaraman^c[Show more](#)  Share  Cite<https://doi.org/10.1016/j.nexres.2025.100961> [Get rights and content](#) 

Abstract

The herbicidal compound [2'-((4,6-dimethoxy-1,3,5-triazin-2-yl)carbonyl)-1,1,6'-trifluoro-N-methylmethanesulfonamide] was systematically investigated to explore its structural, electronic, vibrational, and nonlinear optical (NLO) characteristics. Density Functional Theory (DFT) calculations were carried out at the B3LYP/6-31G(d,p) level, while solvent effects were examined through Time-Dependent DFT (TD-DFT). The computed frontier molecular orbital energies revealed only a slight variation in the HOMO–LUMO energy gap, from 4.8409 eV in the gas phase to 4.9247 eV in chloroform, indicating stability against solvent perturbations. Vibrational analysis identified distinct characteristic modes associated with C–H, SO₂, CH₃, and C–F groups. Natural Bond Orbital (NBO) analysis confirmed strong intramolecular charge-transfer interactions, with a stabilization energy of 49.87 kJ mol⁻¹ from LP(2)→π* delocalization between O₉ and N₁₃–C₂₅. Mulliken charge distribution, supported by Molecular Electrostatic Potential (MEP) mapping, delineated the dominant electrophilic and nucleophilic regions, highlighting probable reactive sites. Molecular docking studies indicated favorable binding with conserved biomolecular regions (–6.7 kcal mol⁻¹), while molecular dynamics simulations reinforced stable interactions with an enhanced binding affinity (–9.6 kcal mol⁻¹). Complementary molecular graph theoretical analyses provided insights

into connectivity indices, electronic delocalization, and their correlation with chemical stability and reactivity. Importantly, the molecule exhibited a high dipole moment (6.83 D), notable polarizability, and significant hyperpolarizability ($\beta_{\text{tot}} = 87.07$ esu), confirming its strong NLO response. These results not only establish the title compound as a structurally stable and electronically active herbicidal compound but also highlight its potential for optoelectronic and photonic device applications.

Introduction

In recent years, herbicides have become increasingly important in modern agriculture, as they are designed to support crop growth by providing a competitive advantage over weeds. [2-((4,6-dimethoxy-1,3,5-triazin-2-yl)carbonyl)-1,1,6'-trifluoro-N-methylmethanesulfonanilide], commonly referred to as DMT-TF-MSA, belongs to the chemical class of pyrimidinyl (thio)benzoates. It is widely employed in agricultural practices, particularly in rice cultivation, for the effective control of a broad spectrum of weeds. It is an acetolactate synthase inhibitor (ALS), which means it inhibits the enzyme acetolactate synthase essential for plant biosynthesis of branched-chain amino acids [1]. DMT-TF-MSA inhibits the growth of susceptible weed species by inhibiting acetolactate synthase. As with other ALS inhibitors, resistance management is crucial to their use, as biotypes can develop resistance when herbicides with the same mode of action are applied too frequently. Herbicides are utilized in Winland ecosystems, aquatic environments, and forests to control weeds and maintain aesthetic appearance [2]. They can be organized into multiple categories, such as non-selective herbicides and selective herbicides, chemical structure, mechanism of action, and length of persistence in soil, among others. For example, DMT-TF-MSA is one herbicide formed from microorganisms, plant-incorporated protectants, and natural substances (essential oils) [3]. There is some concern that long-term exposure to herbicides like DMT-TF-MSA, particularly among at-risk populations, may have chronic health effects, including neurotoxicity and disability outcomes [4]. DMT-TF-MSA, chemical formula of $C_{14}H_{13}F_3N_4O_5S$ and a molecular mass of 406.34 g/mol. Structurally, DMT-TF-MSA is made up of a triazine ring with a sulfonanilide group with 12 and 7 hydrogen bond acceptors and rotatable bonds, respectively [5]. DMT-TF-MSA can control a wide range of weeds by inhibiting acetolactate synthase, which is essential for the synthesis of branched-chain amino acids crucial for plant growth [6].

Density Functional Theory (DFT) is a computational method that is extremely popular due to its potential to provide accurate and efficient simulations that can model atoms and molecules over time, and give us insight into their physical properties and dynamic behavior [7,8]. In the literature, triazine herbicides atrazine, simetryn, and prometryn have been observed experimentally (Raman) and theoretically (DFT) with respect to spectroscopic characterization [9]. The present work aims to provide a comprehensive quantum chemical and molecular-level characterization of the (2-((4,6-dimethoxy-1,3,5-triazin-2-yl)carbonyl)-1,1,6'-trifluoro-N-methylmethanesulfonanilide). The nature of the work is to help establish the structural, electronic, and vibrational characteristics of the

molecule, with completed Density Functional Theory (DFT) calculations at the B3LYP/6-31G(d,p) level [10]. In addition, Time-Dependent DFT (TD-DFT) calculations were completed to establish the solvent effect on the electronic transitions. To help identify stabilization interactions, charge delocalization, reactive sites, and charge distributions, Natural Bond Orbital (NBO) analysis, Mulliken population analysis, and Molecular Electrostatic Potential (MEP) analysis were calculated.

Additionally, molecular docking and molecular dynamics (MD) calculations were used to establish the binding affinity of DMT-TF-MSA to potential biomolecular sites and to create a perspective on biological stability or biological interactions with the target biomolecules [11]. Furthermore, it described the molecular graphing techniques used to study the connectivity indices and sites of electronic delocalization, which contributed to a better understanding of the stability and reactivity characteristics associated with DMT-TF-MSA [12]. The nonlinear optical (NLO) properties of DMT-TF-MSA were theoretically investigated using DFT through the calculation of dipole moment, polarizability, and first hyperpolarizability. The results suggest that the compound exhibits significant potential for advanced optoelectronic and photonic applications, including optical switches, modulators, second-harmonic generation, frequency doubling, multifunctional organic semiconductors, nanomaterials, molecular sensors, biosensing devices, organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and organic photovoltaics (OPVs) [[13], [14], [15]].

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Computational details

The quantum chemical simulation of DMT-TF-MSA was carried out with the DFT approach combined with the B3LYP level of theory using a 6-31G(d,p) basis set [[16], [17], [18]]. The time-dependent DFT and gauge-invariant atomic orbital were used to calculate the electronic spectrum, FMO, and isotropic chemical shielding of DMT-TF-MSA [[19], [20], [21], [22]]. In addition, the NBO, NMR, NLO, Mulliken, and MEP were also simulated using a similar computational approach [[23], [24], [25], [26], [27], ...

Conclusion

This study presents a comprehensive quantum chemical and molecular investigation of DMT-TF-MSA. Geometry optimization and vibrational analysis confirmed the structural stability of the molecule, while calculated chemical shifts reflected shielding effects consistent with electronic delocalization. Natural Bond Orbital (NBO) analysis, Mulliken charge distribution, and Molecular Electrostatic Potential (MEP) mapping revealed distinct regions of electrophilicity and nucleophilicity, providing ...

CRediT authorship contribution statement

L. Sasikala: Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft. **M. Prabhakaran:** Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **P. Rajesh:** Conceptualization, Data curation, Investigation. **G. Jayaraman:** Data curation, Methodology. ...

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. ...

References (57)

P. Jayaprakash *et al.*

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R. Bauernschmitt *et al.*

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Chem. Phys. Lett. (1996)



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