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# Synthesis and antioxidant activity of gallic acid based fluorescent benzothiazole analogue: Photophysical, electrochemical, conceptual DFT, QTAIM and docking investigations

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ABSTRACT

The present investigation reports on the synthesis of a novel 3,4,5-trihydroxy-N-(6-methoxy benzo[d]thiazol-2-yl)benzamide (TMTB) molecule and employs elemental analysis, $^{1}$H NMR, $^{13}$C NMR, and mass spectrum methods to determine the structure of the desired product. The experimental and theoretical absorption and emission spectra of the molecules are used to study the photophysical properties of the TMTB molecule. We investigate the *in vitro* antioxidant activity of TMTB using DPPH and superoxide radical scavenging assays, as well as molecular docking experiments with the target NAD(P)H oxidase (PDB ID: 2CDU) protein. To ascertain the energies of the LUMO and HOMO levels, NLO behaviour, intermolecular charge transport facilitated by global chemical reactivity descriptors, molecular electrostatic potentials (MEP), and hyperpolarizability analyses, an investigation was carried out on their conceptual DFT and QTAIM analyses operating under B3LYP/6–31 G. The simulated DFT calculation shows that TMTB is highly polarizable in both the gas and solvent phases, with HOMO-LUMO energy gaps of 4.18 and 4.24 eV, respectively. Total first and second hyperpolarizability values for TMTB in the gas phase were determined to be 155.09 × $10^{-30}$ and 3611.59 × $10^{-36}$ esu, respectively, whereas in the DMSO phase the values were 556.15 × $10^{-30}$ and 6223.79 × $10^{-36}$ esu. Computational studies results corroborate the experimental findings. Based on the photophysical and computational findings, the newly reported TMTB molecule was determined to be a promising candidate for additional optimization and use in optoelectronic devices.

## 1. Introduction

Biological systems exhibit a remarkable level of dynamism, with processes occurring spontaneously and swiftly within them. Fluorescent small molecules, a significant component of chemical biology, provide efficient tools for viewing biological processes. Since the discovery of the first organic fluorophore [1], numerous theoretical and synthetic attempts have been made to modulate luminous substances. Understanding these quick and intricate biological processes at the molecular level necessitates the use of specialized instruments. Over the last 20 years, research on the design of new small organic fluorescent compounds has produced recommendations for the creation of probes for biological applications, such as biosensing and bioimaging [2,3]. A systematic and complementary approach can tailor the photophysical and electrochemical characteristics of new fluorophores, facilitated by the nature of the electron donor-acceptor groups, substituents, and π-connectors [4]. Because of their many physiological activities, heterocyclic molecules like benzothiazole are particularly important in organic chemistry and drug discovery [5]. Benzothiazole is one of many useful compounds, it is a physiologically relevant heterocycle that has

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