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RESEARCH ARTICLE

Synthesis, Characterization, Antioxidant Properties, and Structural Optimization of a Schiff Base Derived from 4H-1,2,4-triazole-3,5-diamine

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ABSTRACT

Schiff bases were synthesized to explore their potential as effective antioxidant agents. The synthesis involved the condensation of aromatic aldehydes with 4H-1,2,4-triazole-3,5-diamine. The structures of the resulting compounds were confirmed using various spectroscopic techniques and elemental analysis. Furthermore, theoretical studies, including in silico computations with Density Functional Theory (DFT) calculations, supported the efficiency and stability of the synthesized compounds. The antioxidant activity of the samples was evaluated using the DPPH radical scavenging method, which indicated that the compounds exhibited good antioxidant properties.

Keywords: Antioxidant, Heterocyclic, Schiff Base, Triazole

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1. Introduction

Heterocyclic compounds are a significant category of organic substances characterized by molecular structures that predominantly feature five- or six-membered rings with at least one heteroatom [1]. The most common heteroatoms found in these compounds are oxygen, nitrogen, and sulfur [2]. Triazoles, in particular, are five-membered heterocyclic structures consisting of three nitrogen and two carbon atoms [3]. Triazoles exist in two isomeric forms: 1,2,4-triazole and 1,2,3-triazole, each containing one nitrogen atom resembling that of pyrrole and two nitrogen atoms akin to those found in pyridine. A variety of derivatives of 1,2,4-triazoles exhibit a broad spectrum of biological activities, corresponding to numerous bioactive compounds within their molecular frameworks [4]. These compounds have been associated with a wide range of therapeutic properties, including antibacterial [5], antifungal [6], anti-inflammatory [7,8], antiviral [9,10], antitubercular [11], anticonvulsant [12], antidepressant [3,4], antioxidant [15,16], anticancer [17], and analgesic activities [18,19]. Schiff bases are defined as compounds containing an azomethine group (–C=N–) [20]. They are typically synthesized via a condensation reaction between a primary amine and a carbonyl compound [21]. Schiff bases exhibit a diverse array of biological activities [22]. Antioxidants inhibit the oxidation of other substances [23]. Oxidation is a chemical reaction involving the transfer of electrons or hydrogen atoms from one species (the donor) to another, typically resulting in the oxidation of the donor

species. [24]. Oxidation processes can generate free radicals that can inflict damage or induce cell death. Antioxidants are recognized for their vital role as bioactive agents, providing numerous health benefits and preventing oxidative rancidity in various food items [25].

2. EXPERIMETAL

All chemicals and solvents were sourced from Aldrich and Merck Chemical Companies. Thin-layer chromatography (TLC) was performed using Merck silica gel (60F254) plates with a thickness of 0.25 mm. Melting points were determined using a Stuart SMP3 apparatus. The FT-IR spectra (KBr disk) were acquired on a Shimadzu spectrophotometer in the range 400-4000 cm^{-1}. DMSO was used as the solvent for the Bruker 500 MHz proton NMR recording. An elemental analyzer (Eurovector EA-3000 A) was used for elemental analysis (C, H, and N).

2.1. Synthesis of the compound (1)

4H-1,2,4-triazole-3,5-diamine (0.99 g, 0.01 mol) was combined with 3-hydroxy-4-methoxybenzaldehyde (3.04 g, 0.02 mol) in 25 mL of absolute ethanol, to which two drops of ACOOH were added. The resulting mixture was then refluxed for approximately 2 h. The orange solid product obtained was recrystallized from absolute ethanol, yielding the title compound with an efficiency of (78%); melting point: d> 220°C.

2.2. Synthesis of the compound (2)

A combination of 4H-1,2,4-triazole-3,5-diamine (0.99 g, 0.01 mol) and 3-hydroxy-4-methoxybenzaldehyde (3.04 g, 0.02 mol) was prepared in 25 mL of ethanol, to which two drops of ACOOH were added. The resulting mixture was refluxed for approximately 2 hours. The yellow solid product obtained was purified by recrystallization from absolute ethanol, yielding the title compound (81%); melting point: d > 220°C.

2.3. Anti-oxidant activity procedure:

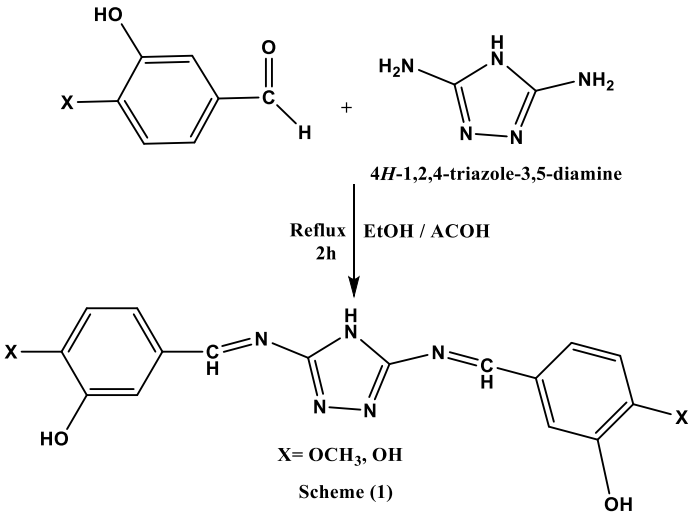
The free radical-scavenging DPPH (2,2-diphenyl-1-picrylhydrazyl) method was employed to assess the antioxidant activity of each sample. In this procedure, 2.5 ml of a 2 mM DPPH solution was combined with 0.5 ml of the synthesized compounds and ascorbic acid at different concentrations (50, 100, and 200 µg/ml). The samples were vigorously mixed and incubated for 30 min in the dark. Absorbance was measured at 517 nm using UV spectrophotometry. Antioxidant activity was calculated using Equation (1).

Percentage inhibition = [(A0-A1)/A0]x100 …… × (1)

where A0 represents the absorbance of the control without the sample, and A1 represents the absorbance of the control with the sample. Antioxidant activity data are expressed as IC50 values (µg/mL), which indicate the concentration required to reduce the effective concentration of DPPH radicals by half. In this study, compound (1) exhibited antioxidant activity similar to that of ascorbic acid, whereas compound (2) showed lower activity. The IC50 values for ascorbic acid, compound (1), and compound (2) at different concentrations (50, 100, and 200 µg/mL) were recorded, with lower IC50 values corresponding to higher antioxidant activities [26].

3. RESULTS &DISCUSSION

The title compounds were synthesized by condensation 4H-1,2,4-triazole-3,5-diamine with 3-hydroxy-4-methoxybenzaldehyde and 3-hydroxy-4-methoxybenzaldehyde as shown in scheme (1). They were characterized using elemental analyses and spectroscopic techniques.



Scheme (1)

The experimental values of micro analysis are agreed with theoretical values as shown in table (1)

Table 1. some physical properties

formula	Molecular mass	color	m.p °C	%Yield
$C_{18}H_{17}N_5O_4$	367	Yellow	220	78
$C_{16}H_{13}N_5O_7$	339	Pale yellowish	230	81

Based on the physical properties of the two compounds shown in Table (1), they are crystalline solids with high melting points. The slight color difference indicates a difference in the electronic environments between compound (1) and compound (2), while the yield indicates ideal reaction conditions and a minimal amount of byproducts.

3.1. FT.IR spectra:

FT-IR spectral data are listed in Table (1) and shown in figures (1 and 2). The broad bands at (3396–3400) cm^{-1} for (O-H) groups, another strong bands at (3135-3187) cm^{-1} for (N-H) groups in the triazole ring. The strong band of the stretching vibration frequency for the azomethine groups (C=N) in the Schiff bases at (1606-1617) cm^{-1}. The bands at (1580-1590) cm-1 are for (C=C) groups.

Table 2. FTIR frequencies in cm^{-1} of the synthesized compounds

compound	ν (O-H)	ν (N-H)	ν (C-H) Aro.	ν (C=N)	ν (C=C)
Comp. (1)	3381	3135	3042	1606	1580
Comp. (2)	3380	3187	3030	1617	1590

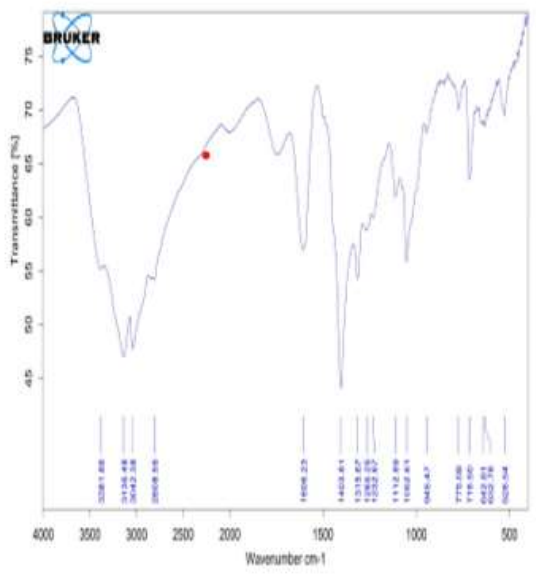


Figure 1. FTIR spectrum of the compound (1)

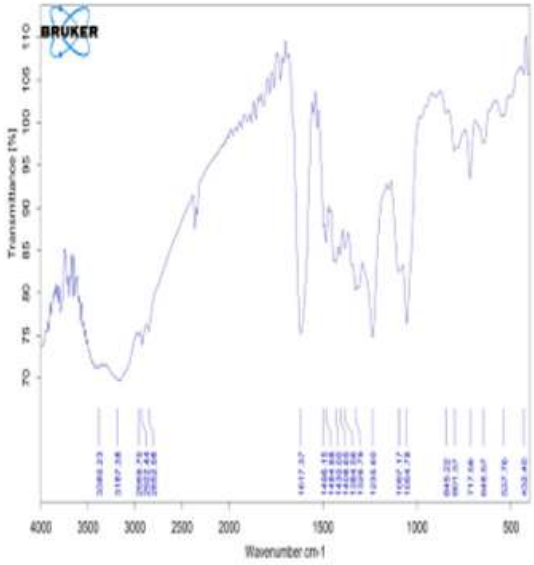


Figure 2. FTIR spectrum of the compound (2)

3.1.1. ^{1}H NMR spectrum of the compound (1)

The 1H NMR spectra of the synthesized compounds were recorded using the solvent (d_6-DMSO). The peaks at (2.51 and 3.35) ppm correspond to the protons of the solvent and water, respectively. The spectrum exhibits chemical shifts (ppm) at 3.82 (s, 6H) for the proton of the methoxy group, 6.88-7.39(m, 6H) for the proton of the aromatic group, 8.94 (s, 2H) for the proton of the azomethine group, 11.43(s, 2H) for the proton of the phenolic group, and 13.33(s, 1H) for the proton of the (N-H) group in the triazole ring. As shown in figure (3)

3.1.2. ^{1}H NMR spectrum of the compound (2)

The spectrum of ^{1}H NMR for the synthesized compounds was recorded utilizing in solvent (d_6-DMSO). The peaks at (2.52 and 3.39) ppm correspond to the protons of the solvent and water, respectively. The spectrum exhibits chemical shifts (ppm) at: 6.81-7.35(m, 6H) for the proton of the aromatic group, 9.45 (s, 2H) for the proton of the azomethine group, 11.20 and 12.47 (s, 2H) for the proton of the two phenolic groups, and 14.31(s, 1H) for the proton of the (N-H) group in the triazole ring. This is shown in figure (4).

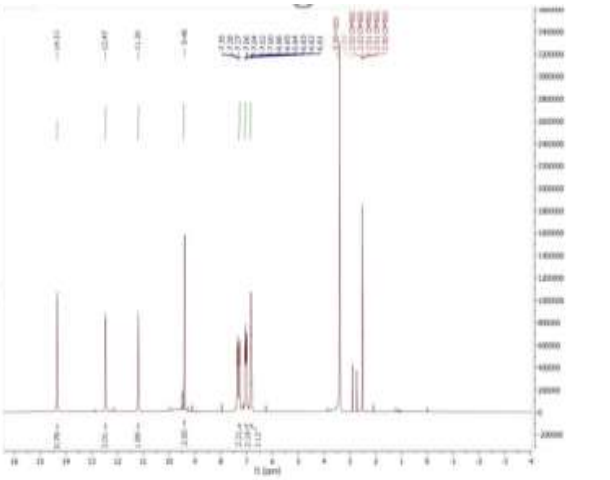


Figure (4) ^{1}H NMR spectrum of the compound (2)

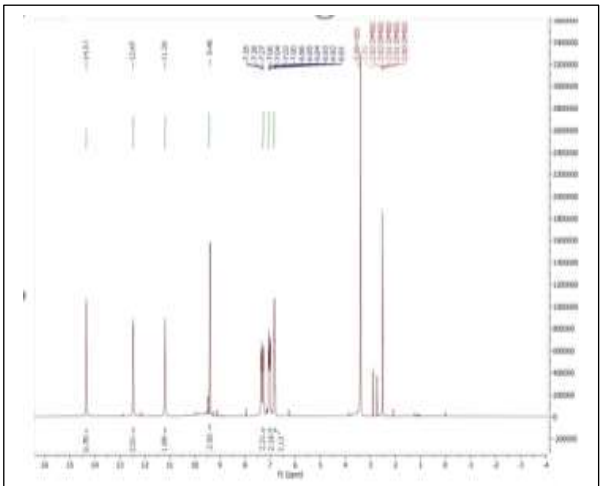


Figure (4) ^{1}H NMR spectrum of the compound (2)

3.2. Mass spectra:

The mass spectrum of compound (1) exhibited a molecular ion peak at (368) m/z and a base peak at (222) m/z, confirming the proposed formula [$C_{18}H_{17}N_5O_4$] for the synthesized compounds. This is shown in figure (5) and Scheme (2).

The mass spectrum of compound (2) exhibited a molecular ion peak at (339) m/z and a base peak at (222) m/z, confirming the proposed formula [$C_{16}H_{13}N_5O_4$] for the synthesized compounds. As shown in figure (6) and Scheme (2).

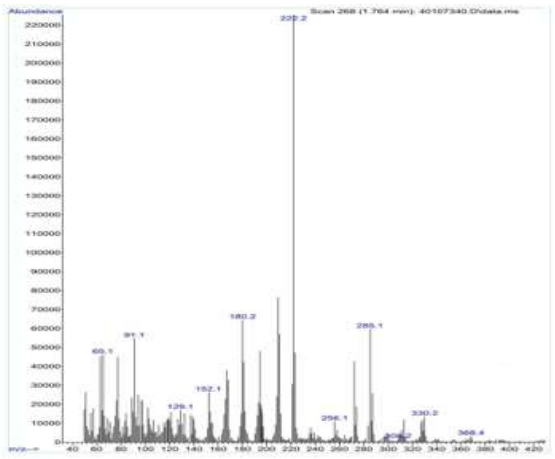


Figure (5) mass spectrum of the compound (1)

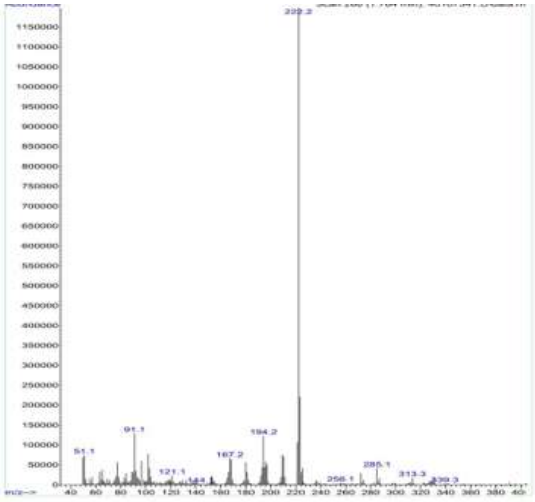
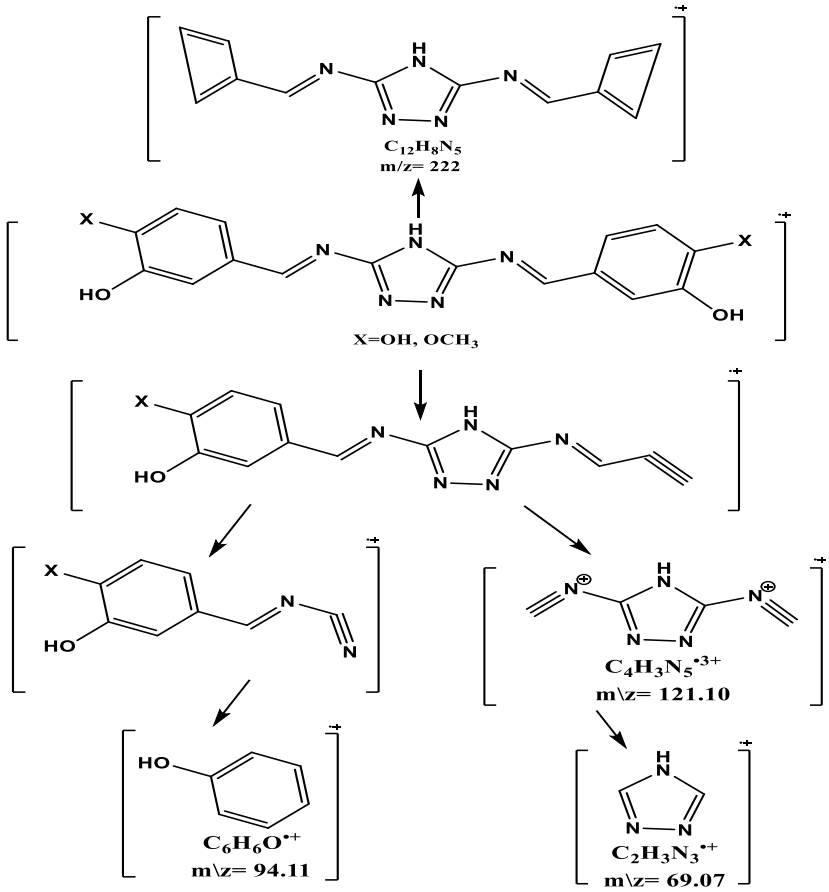


Figure (6) mass spectrum of the compound (2)



Scheme (2) the difragmentation of the comp(1) and comp(2)

3.3. Anti-Oxidant Activity Evalution:

Antioxidant characteristics, especially radical scavenging activities, are significant because they eliminate damaging free radicals in biological systems. DPPH · has been frequently used to investigate the free radical scavenging performance of several antioxidant compounds. The DPPH method was used to evaluate the antioxidant activity of the newly synthesized compounds and standard antioxidants (ascorbic acid) at various concentrations (50, 100, and 200 µg/ml) [27]. The number of electrons collected depends on the reaction, which is distinguished by a change in the deep violet hue (DPPH) or by color fading. By referring to Table (3) and Figure (7), which present the values of antioxidant activity inhibition and the corresponding IC50 values, it can be observed that the highest antioxidant activity values correspond to the lowest IC50 values [28]. When comparing the antioxidant activities of the compounds with ascorbic acid, we found that compound (1) had an activity similar to that of ascorbic acid, whereas compound (2) had a lower activity.

Table 3. data of antioxidant activity for the compounds (1) and (2)

Concentration µg/ml	Ascorbic acid		Comp (1)		Comp (2)	
	% inhib.	IC50	% inhib.	IC50	% inhib.	IC50
50	68		65		54	
100	74	35	72	38	67	42
200	84		77		71	

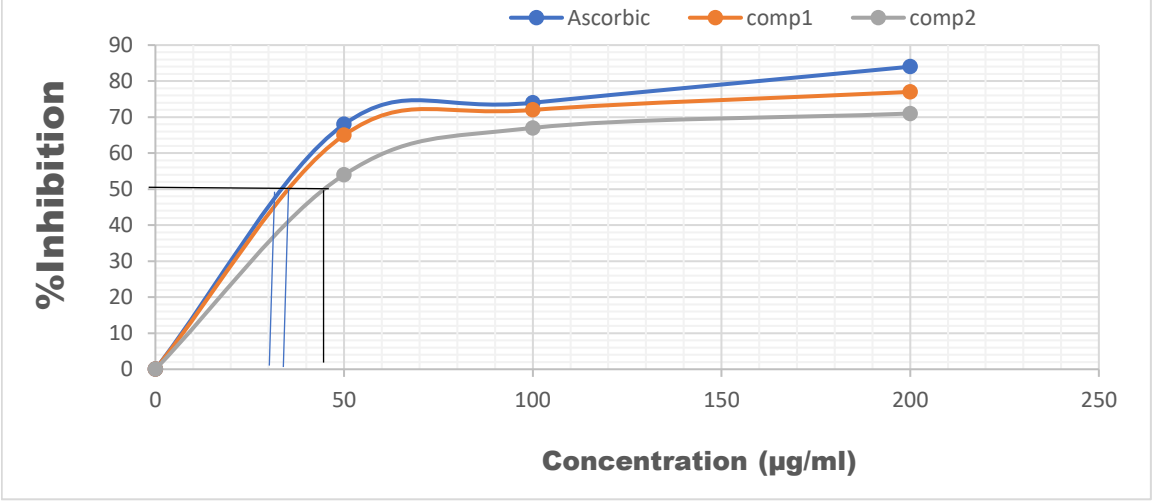


Figure 7. antioxidant activity for the compounds (1) and (2)

3.4. Theoretical study

The Calculations of the theoretical study were performed using the density functional theory (DFT) method at the B3LYP level with a 6-31+G (d,p) bases set using Gaussian (09) programs [29]. The geometry optimization for the ligand and its complexes focuses on the local minimum of each structure with the lowest energy level, as shown in Figures (8 and 9). The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) were computed the B3LYP / 6-31+G (d,p) level, as shown in Fig. (8 and 9),. The values of EHOMO, ELUMO and Energy gap (ΔE) are displayed in Table (4). The capacity of a molecule to interact with other molecules is generally represented by the values of the energies (EHOMO and ELUMO) of the molecular orbitals [30]. The electron-donating capability of a molecule is explained by the term EHOMO. A molecule with a high EHOMO value has a strong capacity to donate electrons to a lower-energy molecule (an empty orbital). The capacity of a molecule to receive electrons from an energetic molecule is

greatest when it has a low ELUMO value (an unoccupied orbital)19. The energy gap (ΔE) was calculated) by using Equation (2)[31]. The global reactivity descriptors include absolute electronegativity (χ), chemical potential (Pi), absolute hardness (η), absolute softness (σ), global electrophilicity (ω), and global softness (S). Chemically reactive molecules exhibit a low HOMO-LUMO gap [32]. The theoretical results were consistent with the findings of the antioxidant examination. The energy gap of comp(1) is less of the energy gap of comp(2) so that comp(1) is more reactive, That is agreeable with the activity of antioxidant

Table 4. quantum chemical parameters

parameters	Comp1	Comp2	Equation
EHOMO (eV)	-5.3911173	-5.4041781	ΔE = ELUMO−EHOMO …… 2
ELUMO (eV)	-1.8715038	-1.8679665	
Δ E (eV)	3.5196135	3.5362116	χ = − (EHOMO +ELUMO)/2 ……3
χ (eV)	3.63131055	3.6360723	η = (ELUMO – EHOMO) /2 4
η (eV)	1.75980675	1.7681058	σ = 1/η …….5
σ $(eV)^{-1}$	0.568244212	0.565577015	S= 1/2η …….6
Pi (eV)	-3.63131055	-3.6360723	
S $(eV)^{-1}$	0.879903375	0.8840529	Pi= −χ ……..7
ω (eV)	-3.195202409	-3.214480261	ω=Pi/2η ……8

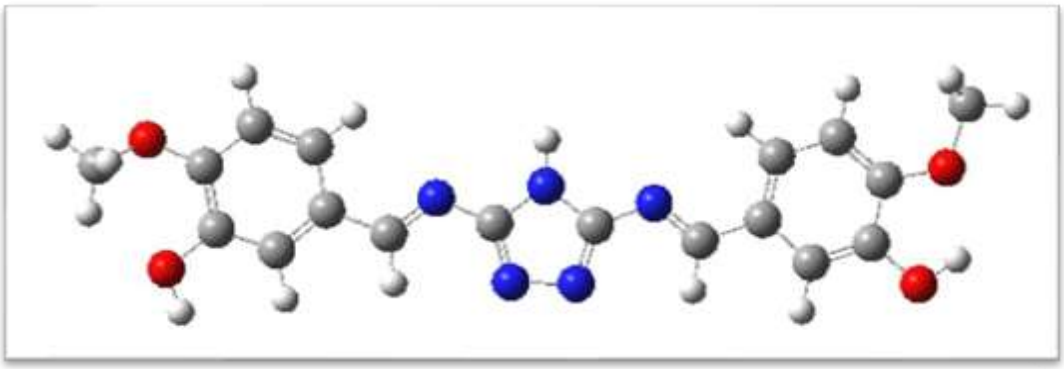


Figure 8. the geometry optimization HOMO and LUMO of compound (1)

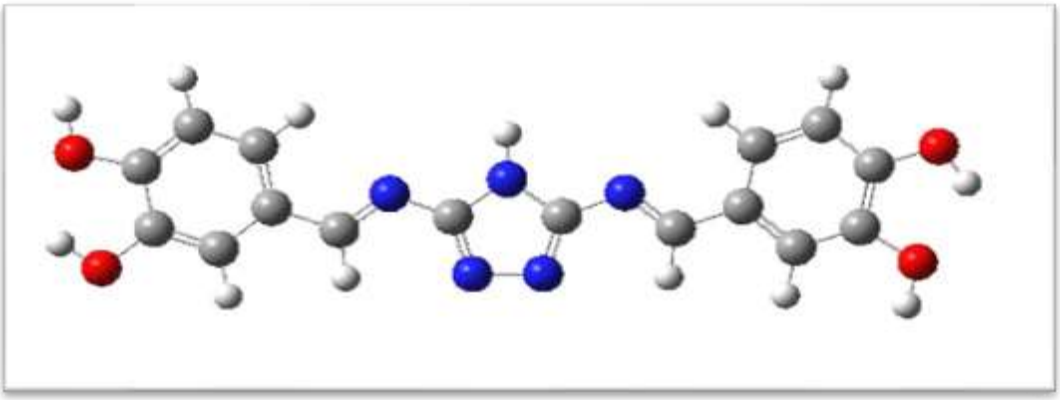


Figure 9. the geometry optimization HOMO and LUMO of compound (2)

4. Conclusion

Two compounds of 1,2,4-triazole derivatives were synthesized and characterized by macro analysis, FT-IR, ^{1}H-NMR, and mass spectroscopy. The final part of this research involved evaluating the antioxidant

activity of these compounds through their ability to inhibit DPPH radical scavenging. The compounds exhibited good antioxidant activity. The theoretical study is in agreement with the antioxidant activity.

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