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DFT-Based Mechanistic Study and QSAR Modeling of Antioxidant Activity of Triazole Derivatives

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ABSTRACT

Triazole-derived compounds are known to exhibit a variety of favourable biological activities, including antioxidant, anti-inflammatory, and antibacterial activities. Research on the potential of these compounds as antioxidant compounds was carried out theoretically through analysis of global reactivity parameters and measurement of antioxidant activity. The Density Functional Theory (DFT) method was used to study the molecular structure, global reactivity parameters, and hydrogen-atom release mechanism by calculating BDE, IP, PDE, PA, and ETE values. Antioxidant activity was expressed as the Inhibition Concentration 50% (IC50) values obtained from multilinear regression-based Quantitative Structure-Activity Relationship (QSAR) analysis. Validation was performed by comparing theoretical IC50 values with experimental values. The results show that molecule A is the most reactive, followed by molecules B, D, and C, which have the same theoretical IC50 value as the experiment. The interaction of the compounds with ROS and RNS radicals exhibited spontaneous reactions with negative ?G, reinforcing their potential antioxidant activity. This study confirmed that triazole-derived compounds have the potential to be further developed as effective antioxidants.

Contribution to Sustainable Development Goals (SDGs):
SDG 2 – Zero Hunger
SDG 3 – Good Health and Well-Being
SDG 12 – Responsible Consumption and Production

1. INTRODUCTION

Every living organism produces free radicals within its body as a result of ongoing biochemical reactions. These free radicals cause a chain reaction of oxidative reactions that continuously generate free radicals, leading to the formation of Reactive Oxygen Species (ROS). ROS are highly reactive free radicals, byproducts of the body's metabolism, can cause damage to body cells [1].

Antioxidants are compounds capable of protecting cells from damage caused by free radicals [2]. Antioxidants bind to free radicals and donate electrons, thereby halting the oxidative chain reaction because the free radical molecules have reached stability [3].

One compound rich in antioxidants is triazole. Triazole compounds exhibit various pharmacological activities. Various drugs containing triazoles prove their pharmacological significance, such as antimalarial, antimicrobial, antitumor, antiviral, antiproliferative, anticancer, antioxidant, analgesic, antibacterial, and antidiabetic. Triazole compounds are known to have good cytotoxic activity, as research conducted by Gupta *et al.*, they found that triazole compounds are effective therapeutic elements by improving pharmacokinetics and physicochemical features [4].

Excellent effectiveness of the DFT method in structural studies to determine the mechanism of antioxidant reactions, anticancer activity, and various quantum parameters related to antioxidant activity and toxicity has been widely reported by various literature. The DFT method is used because the accuracy of its calculations is close to experimental results [5]. Several theoretical studies of antioxidant activity using the DT method include antioxidant predictions in atronorin compounds [6], antioxidant capacity and toxicity of anthocyanidin compounds [5], antioxidant potential of ferulic acid [7], and others. The results of theoretical analysis using the DFT method provide relatively similar results to the experiments.

Based on this background, this study aims to theoretically explore the antioxidant activity of triazole derivatives using DFT calculations. This study also aims to compare theoretical calculations with experimental data to assess the model's suitability and evaluate the potential of these compounds as effective antioxidants.

2. MATERIALS AND METHODS

This research is a theoretical research that will be carried out in the Computing Laboratory, Department of Chemistry, Faculty of Mathematics and Natural Sciences, Andalas University. The equipment used in this research, namely a set of PC/Laptop, the Gaussian 16 W program package, and SPSS V.27 software. The molecular model analyzed is the molecular structure of a triazole derivative compound shown in Figure 3.1:

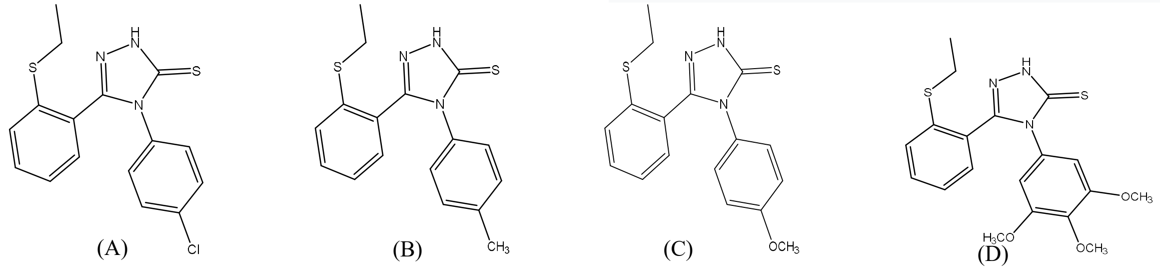

Fig. 1. Structure of triazol molecules
(A) 4-(4-chlorophenyl)-5-(2-(ethylthio)phenyl)-2,4-dihydro-3 *H* -1,2,4-triazol-3-thione
(B)5-(2-(ethylthio)phenyl)-4-(*p* -tolyl)-2,4-dihydro-3 *H* -1,2,4-triazol-3-thione
(C)5-(2-(ethylthio)phenyl)-4-(4-methoxyphenyl)-2,4-dihydro-3 *H* -1,2,4-triazol-3-thione0
(D)5-(2-(ethylthio)phenyl)-4-(3,4,5-trimethoxyphenyl)-2,4-dihydro-3 *H* -1,2,4-triazol-3-thione

2.1. *Optimization of Molecular Structure Geometry*

The molecular structure of the triazole derivative compound was depicted and observed using Gauss View 6.0, then molecular optimization was carried out using Gaussian 16W software using the DFT calculation method with the B3LYP/6-31G basis sets. The results of the most stable triazole derivative compound structure optimization were proven by obtaining the lowest total energy from the observed structure [8]. The results of the geometry optimization were in the form of optimal geometry structures and notepad.

Triazole derivative compounds are symbolized by ArRNH. The molecules to be optimized are ArRNH, ArRN•, ArRN H•+, ArRN$^-$. The resulting output is in the form of optimal geometric structures, Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) contours, HOMO Energy (E_{HOMO}), LUMO Energy (E_{LUMO}), UV-Vis spectrum, and formation enthalpy (ΔH_f). The results of the ΔH_F calculation are then determined by the BDE, IP, PDE, PA, and ETE values, and the antioxidant reaction mechanism with suitable radicals from triazole derivative compounds.

2.2. *Determining the Parameter Values for Global Reactivity Analysis*

Descriptive parameters that will indicate the reactivity of a molecule can use the parameters Electrophilicity (ω), Nucleophilicity (Ɛ), Ionization Energy (I), Electron Affinity (A), Bandgap (ΔE), Electronegativity (X), Chemical Potential (μ), Hardness (η), Softness (σ). The calculation of the value of these parameters can be seen from the formulas below [8] :

$$I = E_{HOMO}, \quad A = -E_{LUMO},$$

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

$$X = \frac{-E_{HOMO} - E_{LUMO}}{2}, \quad \mu = \frac{E_{HOMO} + E_{LUMO}}{2},$$

$$\eta = \frac{E_{LUMO} - E_{HOMO}}{2}, \quad \sigma = \frac{1}{\eta}$$

$$\omega = \frac{X^2}{2\eta} = \frac{\mu}{4}, \quad \varepsilon = \frac{1}{\omega}$$

Based on the parameter values above, the reactivity of triazole derivatives and their derivatives as antioxidants was then analyzed.

2.3. *Determining the Antioxidant Activity Value of Triazole Derivative Compounds*

The antioxidant activity of triazole derivative compounds is expressed in IC_{50} values. The determination of the IC_{50} value was carried out using the Quantitative Structure and Activity Relationship (QSAR) method using SPSS 27 software which is based on a multilinear regression equation. In this analysis, the experimentally obtained IC_{50} value acts as the dependent variable, and the BDE, IP, PDE, PA, and ETE values act as independent variables that will produce the best selected regression equation. Based on the analysis of these results, the theoretically predicted IC_{50} value will be obtained.

The analysis of the reaction mechanism of antioxidant inhibition against radicals is theoretically determined through three reaction mechanisms, namely [6]:

1. Hydrogen Atom Transfer (HAT) Mechanism

$$ArOH + R\bullet \rightarrow ArO\bullet + RH \qquad (1)$$

The enthalpy of this reaction is Bond Dissotiation Energy (BDE).

2. Single Electron Transfer-Proton Transfer (SET-PT) Mechanism

a. Single Electron Transfer (SET)

$$R\bullet + ArO\bullet\bullet H \rightarrow R- + ArOH^{+\bullet} \qquad (2)$$

The associated reaction enthalpy is the ionization potential (IP).

b. Proton Transfer (PT)

$$ArOH\bullet+ \ \rightarrow ArO\bullet + H^{+} \qquad (3)$$

The associated reaction enthalpy is Proton Dissociation Energy (PDE).

3. Sequential Proton Loss Electron Transfer (SPLET) Mechanism

a. Sequential Proton Loss (SPL)

$$ArOH \rightarrow ArO^{-} + H^{+} \qquad (4)$$

The associated reaction enthalpy is Proton Affinity (PA).

b. Electron Transfer (ET)

$$ArO- + R\bullet \rightarrow ArO\bullet + R^{-} \qquad (5)$$

The associated reaction enthalpy is Electron Transfer Energy (ETE).

The best mechanism is determined by the smallest enthalpy value. The numerical enthalpy parameters can be calculated using the following equation:

$$BDE = \Delta H_f\,(ArO^{\bullet}) + \Delta H_f(H^{\bullet}) - \Delta H_f\,(ArOH) \qquad (6)$$

$$IP = \Delta H_f\,(ArOH^{\bullet+}) + \Delta H_f\,(e^{-}) - \Delta H_f(ArOH) \qquad (7)$$

$$PDE = \Delta H_f\,(ArO^{\bullet}) + \Delta H_f\,(H^{+}) - \Delta H_f\,(ArOH^{\bullet+}) \qquad (8)$$

$$PA = \Delta H_f\,(ArO^{-}) + \Delta H_f\,(H^{+}) - \Delta H_f\,(ArOH) \qquad (9)$$

$$ETE = \Delta H_f\,(ArO^{\bullet}) + \Delta H_f\,(e^{-}) - \Delta H_f\,(ArO^{-}) \qquad (10)$$

In this study, the symbol ArOH is replaced with ArNH.

2.4. *Determining the Reaction of Triazole Derivative Compounds with ROS/RNS Radical Representatives*

As a further test, a study was conducted on the reaction of triazole derivative compounds to radicals representing ros/rns. Examples of representative free radicals are the radicals (OH •) and (NO •) [9]. The Δg value for hydrogen abstraction from the most reactive OH bond of the studied compounds was calculated in the gas phase. The results obtained were in the form of a compound reaction with a more reactive radical towards ros/rns which was determined from the ΔG(-) value.

3. RESULT AND DISCUSSION

3.1. *Frontier Molecular Orbital Analysis of Triazole Derivative Compounds*

Frontier molecular orbital analysis predicts the reactive properties of a molecule, focusing on the HOMO and LUMO. The HOMO acts as an electron donor and is a nucleophile, while the LUMO acts as an electron acceptor and is an electrophile [10]. The partial distribution of electrons in these two orbitals can be understood through the visualization of the HOMO and LUMO contours. The LUMO-HOMO energy gap, or bandgap energy, is also important to see the reactivity of the molecule; the smaller the bandgap, the longer the π electron conjugation, and the more reactive the molecule becomes [11]. Visualization of the HOMO and LUMO contours of triazole derivatives in the gas phase is shown in Figure 2.

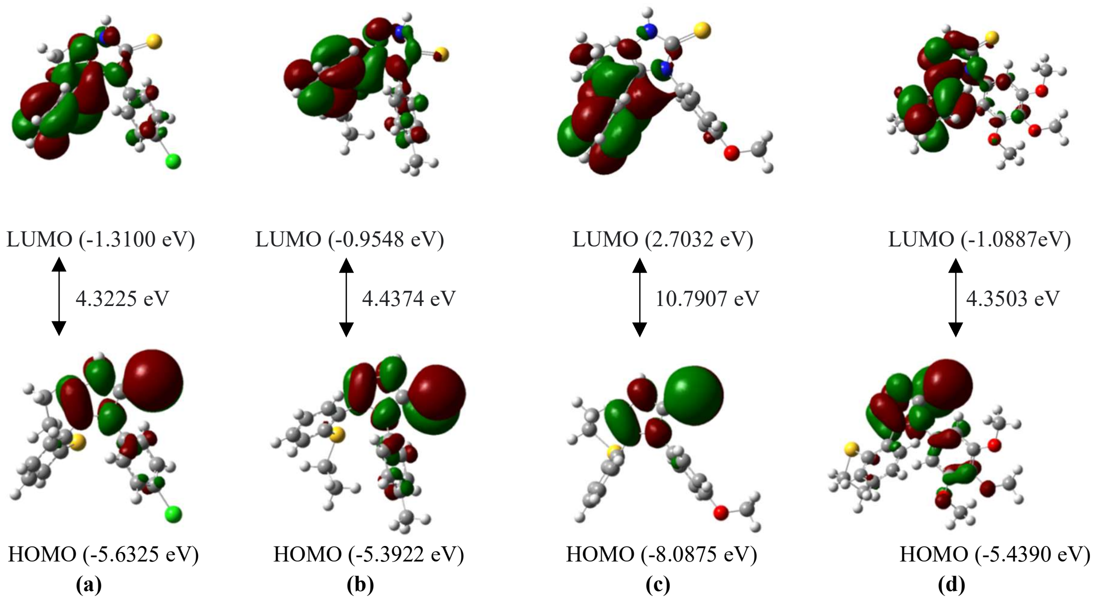

Fig. 2. HOMO and LUMO contours of triazole derivative molecules. (green = bonding orbital electron density, red = anti-bonding orbital electron density

The HOMO contour map shows the region of the molecule that acts as an electron donor, and the LUMO contour map shows the region of the molecule that acts as an electron acceptor. Therefore, it can be concluded from this frontier molecular orbital analysis that the aromatic ring 1 acts as an electron withdrawer and the S atom in the C=S group acts as an electron pusher.

3.2. *Analysis of Global Reactivity Parameters of Triazole Derivative Compounds*

Global reactivity parameter analysis can estimate the reactivity of triazole derivatives as antioxidants. The ease with which a compound reacts with free radicals determines its antioxidant activity. The process begins with the cleavage of the NH bond in the antioxidant compound, forming ArN radicals and H radicals. The H radical reacts with the free radicals, forming a stable neutral molecule [9].

Table 1. Frontier energy, bandgap, and dipole moment of triazole derivative compounds

Compound	E_{HOMO} (eV)	E_{LUMO} (eV)	Bandgap (eV)	Dipole moment (Debye)
Molecule A	-5.6325	-1.3100	4.3225	6.9236
Molecule B	-5,3922	-0.9548	4.4374	**7,1983**
Molecule C	-5,4042	-1.1592	**4,2450**	6.3236
Molecule D	-5.4390	-1.0887	4,3503	4,7689

The bandgap value indicates the reactivity of a molecule, indicating the ability of electron transfer from the HOMO to the LUMO. The smaller the bandgap, the faster the electron transfer process and the more reactive the molecule [10]. Molecule A has the smallest bandgap, indicating the highest reactivity. The dipole moment describes the molecule's ability to separate poles, with a larger dipole moment, the separation of poles is easier, affecting the ease of breaking the H radical in the molecule.

Table 2. Global reactivity parameters of triazole derivative compounds

Reactivity Parameter (eV)	Molecule A	Molecule B	Molecule C	Molecule D
Electronegativity (X)	3,4712	**3,1735**	3,2817	3,2639
Chemical potential (μ)	-3.4712	**-3.1735**	-3,2817	-3.2639
Hardness (η)	2,1613	2,2187	**2.1225**	2,1751
Softness (σ)	0.4627	0.4507	**0.4711**	0.4597
Electrophilicity (ω)	**2.7876**	2,2697	2,5370	2.4488
Nucleophilicity (Ɛ)	**0.3587**	0.4406	0.3942	0.4084
Electron Affinity (A)	**1,3100**	0.9548	1,1592	1,0887
Ionization Energy (I)	5.6325	**5,3922**	5,4042	5,4390

Based on the data obtained, it can be concluded that molecule B is the most reactive molecule compared to other molecules because it has more better reactivity parameters. Good antioxidant activity is characterized by low bandgap, high dipole moment, low electronegativity, high chemical potential, low hardness, high softness, high electrophilicity, low nucleophilicity, high electron affinity, and low ionization energy. Based on the overall analysis of the global reactivity parameters of triazole derivative compounds, the following reactivity results were obtained: molecule B > molecule A > molecule C > molecule D.

3.3. Analysis of Antioxidant Activity Values of Triazole Derivative Compounds

Antioxidant compounds have different activities. Analysis of the mechanism of release of H radical atoms (H•) can help determine their activity. Antioxidant compounds prevent oxidation by donating electrons from the release of H radical atoms (H•), stabilizing free radicals, and forming neutral compounds. Triazole derivative compounds show antioxidant activity by breaking the NH bond, producing H radicals (H•) and ArN radicals (ArN•). The easier the release of H• and the formation of RH molecules, the better the antioxidant activity. The cleavage of NH bonds in triazole derivative compounds is observed in 3 mechanisms, with smaller BDE, IP, PDE, PA, and ETE value parameters indicating unstable and easily broken NH bonds [12]. The easier the cleavage of NH bonds, the easier the inhibition of free radicals. The BDE, IP, PDE, PA, and ETE value parameters can be seen in Table 3.

Table 3. BDE, IP, PDE, PA, and ETE values (kJ/mol) of triazole derivative compounds

Compound	BDE (kJ/mol)	IP (kJ/mol)	PDE (kJ/mol)	PA (kJ/mol)	ETE (kJ/mol)
Molecule A	1686,2563	702,5838	987,8790	**1421,0624**	265,1939
Molecule B	1687,0964	678,9832	1012,3198	1447,0653	**240,0311**
Molecule C	**1685,5106**	668,8120	**775,7570**	1444,5690	245,1482
Molecule D	1687,4088	**438,0542**	1253,5612	1435,6549	251,7539

The energy value of the H radical cleavage in triazole molecules is much higher than the standard N-H bond dissociation energy (usually 300-400 kJ/mol) because this value represents the accumulated energy of the entire molecule and not the single N-H dissociation energy. The information in Table 3 shows that NH bond cleavage occurs more easily through the HAT and SPL-ET mechanisms than the SET-PT mechanism due to the lower BDE values and total PA+ETE energy. Overall, the compound that showed the highest antioxidant activity was molecule C because it had the lowest cleavage energy compared to the other molecules.

A multilinear correlation test using SPSS 27 was performed to evaluate the linear relationship between the experimental IC_{50} values and the theoretical antioxidant activity parameters. This test involved two variables: IC_{50} as the dependent variable and the antioxidant parameters (BDE, IP, PDE, PA, and ETE) as the independent variables.

The best regression equation is selected based on the model that uses the fewest possible independent variables. In this selection, the statistical parameters of each model need to be considered, including the correlation coefficient (R) which must be greater than 0.8, the coefficient of determination (R^2) which must be greater than 0.8, and a small standard deviation (SD)

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compared to the mean [13]. The best equation must meet these criteria and have a specific description.

Table 4. Selected equation parameters on antioxidant activity

No.	Independent Variable	R	R^2	Sig	Mean	Elementary School
1.	BDE, IP, ETE	1	1	0.01	4.3	2,15114

The selected equation for antioxidant activity obtained in Table 4.8 can be stated that antioxidant activity is determined by the BDE, PDE, and ETE values. Based on the results of the multilinear regression analysis which states the relationship between antioxidant activity ($IC_{50)}$ experimentally and the BDE, PDE, and ETE values, the following QSAR equation can be obtained:

Y= 4541.825 + (-2.699) BDE + (-0.009) IP + (0.082) ETE

(n= 4; R^2 = 1; SD= 2.15114)

Table 5. IC_{50} values of triazole derivative compounds for antioxidant activity experimentally and theoretically predicted.

No.	Compound	IC_{50} experimental	IC_{50} theory
1.	Molecule A	5,64 ± 0,003	5,64 ± 0,003
2.	Molecule B	1,51 ± 0,08	1,51 ± 0,08
3.	Molecule C	6,30 ± 0,013	6,30 ± 0,013
24.	Molecule D	3,75 ± 0,001	3,75 ± 0,001

The results of the multilinear regression analysis showed that the theoretical predicted IC_{50} value of the triazole derivative compound was the same as the experimental IC_{50} value, this was indicated by the $R^2 = 1$ in the correlation test with multilinear regression analysis. The $R^2 = 1$ value in antioxidant activity is an ideal and strong relationship between the dependent variable and the independent variable in the best equation selected with a residual value of 0.00 which indicated that there was no difference between the experimental IC_{50} value and the theoretical predicted IC_{50} value.

3.4. Analysis of the Interaction of Triazole Derivative Compounds with ROS/RNS Radical Representatives

The interaction of triazole derivative compounds with ROS/RNS radicals needs to be analyzed because free radicals have an important role in biological life systems. To observe the antiradical activity of triazole derivative compounds, which are exogenous antioxidants, these compounds need to be reacted with (OH•) as a representative of ROS radical agents and (NO•) as a representative of RNS radical agents.

Table 6. Bond lengths, angles, and gibbs free energies (ΔG) formed between radicals and triazole derivative compounds.

No.	Compound	Radical	Bond Length (Å)	Angle(°)	ΔG (kcal/mol)
1.	Molecule A	.OH	1,394	102,345	-75,122
		NO	1,412	113,848	**-129,219**
2.	Molecule B	OH	1,394	102,213	-75,124
		NO	1,429	114,999	-129,218
3.	Molecule C	OH	1,368	106,454	-74,746
		NO	1,356	115,378	-128,541
4.	Molecule D	OH	1,394	102,306	-5,124
		NO	1,430	114,937	-59,217

Table 6 shows that when triazole derivatives release H radicals from the NH bond, reacting with ROS/RNS radicals, the result is a negative or near-zero Gibbs free energy. This indicates that the free radical scavenging reaction by triazole derivatives occurs spontaneously, indicating the antioxidant properties that are reactive to free radicals. A more negative Gibbs free energy indicates a faster reaction [14]. The reaction with NO radicals produces a more negative Gibbs free energy than with OH radicals, influenced by the electronegativity of the radical elements. Steric hindrance by the C=S bond close to the NH bond also affects the Gibbs free energy. The dihedral angle is close to planar and the short bond length indicates the reactivity of triazole derivatives towards radicals. Overall, the data show that triazole derivatives are potential antioxidants with good radical scavenging activity.

4. CONCLUSION

This study shows that molecule B has the highest reactivity based on global reactivity parameters, although molecule C shows the best antioxidant activity based on the energy value of H radical release. The interaction of triazole compounds with OH• and NO• radicals produces negative Gibbs free energy (ΔG) values, indicating that the reaction is spontaneous. These data strengthen the potential of all triazole compounds as antioxidants capable of scavenging free radicals Overall, triazole derivative compounds have great potential to be further developed as effective antioxidant candidates in pharmaceutical or therapeutic applications, with IC_{50} values in the range of 1.50 – 6.30 μg/mL, which shows very strong antioxidant activity.

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