

PREDICTION OF THE STEEL CORROSION INHIBITION POTENTIAL OF TRYPTOPHAN DERIVATIVES BASED ON QUANTUM CHEMICAL PARAMETERS

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Abstract – The corrosion inhibition performance of tryptophan derivatives was investigated using density functional theory calculations. Quantum chemical descriptors were analyzed to assess electron-donating and electron-accepting abilities and interaction tendencies with the Fe surface. Most electron-donating substitutions produced favorable changes in the computed descriptors, although the magnitude and direction of these effects depended on substituent type and position. Among the hydroxyl-substituted derivatives, 4-OH-TN and 6-OH-TN showed the highest estimated inhibition efficiency of 93.61%, while 6-OH-TN exhibited a favorable overall combination of quantum chemical descriptors. Introducing stronger electron-donating groups at the C6 position further improved the predicted inhibition performance. Among the C6-substituted derivatives, 6-NH₂-TN exhibited the most favorable electronic descriptors and the highest estimated inhibition efficiency of 98.75%. These results highlight the roles of substituent type and position in modulating the predicted corrosion inhibition performance of tryptophan derivatives.

Key words – Quantum chemical calculations; corrosion; inhibitors; tryptophan; electron-donating derivatives.

1. Introduction

Metal corrosion has serious impacts on the sustainable development of industries, construction, and transportation. The corrosion process leads to the deterioration of mechanical properties, destruction of material structures, and reduction in equipment service life. It may also cause leakage of hazardous chemicals, thereby increasing the risk of incidents and accidents during operation. To control and mitigate this phenomenon, various corrosion protection methods have been implemented, including protective surface coatings, metal plating, electrochemical protection methods, and the use of materials with high corrosion resistance. Among these approaches, the use of corrosion inhibitors is considered an effective, flexible, and economical solution, particularly in solution systems. Recently, the development of “green” inhibitors derived from environmentally friendly, non-toxic, and biodegradable sources has attracted considerable attention from scientists [1].

Numerous studies have shown that organic compounds containing electron-donating groups, such as –OH, –NH₂, –CH₃, and –OCH₃, exhibit high corrosion inhibition efficiency due to their strong interaction with metal surfaces through both chemical and physical adsorption mechanisms [2]. Electron-donating functional groups,

together with π -conjugated systems in aromatic and heterocyclic rings, can increase the electron density of organic molecules, particularly at active centers such as N, O, and S heteroatoms. This increase in electron density leads to an increase in the energy of the highest occupied molecular orbital (HOMO), thereby enhancing the ability of inhibitor molecules to donate electrons to the vacant orbitals, usually d orbitals, of metals, forming stable coordination bonds.

Among potential organic compounds, tryptophan, an aromatic amino acid, is regarded as a promising “green” corrosion inhibitor owing to its molecular structure containing multiple electron-rich active centers and an extended π -conjugated system. The tryptophan molecule consists of an indole ring, an aromatic heterocycle containing a nitrogen atom, together with –NH₂ and –COOH functional groups, enabling effective interaction with metal surfaces through both chemical and physical adsorption mechanisms. The nitrogen atoms in the indole ring and amino group can donate electrons to the vacant d orbitals of metals, forming coordination bonds, while the π -conjugated system of the indole ring promotes π -d interactions, contributing to the enhanced stability of the protective film. Owing to its non-toxicity, high biodegradability, and significant inhibition efficiency, tryptophan has been widely investigated as a corrosion inhibitor for metals such as steel, copper, and aluminum in acidic media, including HCl and H₂SO₄, at various concentrations [3–5].

However, current studies have mainly focused on the tryptophan molecule itself (TN), whereas the influence of substituents, particularly electron-donating groups, on its corrosion inhibition potential has not yet been systematically investigated. Therefore, in this study, we compare the corrosion inhibition potential of tryptophan and its derivatives containing electron-donating groups using quantum chemical calculations. Electronic and thermodynamic parameters are analyzed to clarify the interaction mechanism between inhibitor molecules and the metal surface, as well as to evaluate the corrosion inhibition tendency and potential of these compounds. Through this theoretical approach, the study aims to guide the design of effective “green” corrosion inhibitors, contributing to the improved protection of steel in corrosive environments.

2. Methods

In this study, density functional theory (DFT) was employed as the main theoretical tool to investigate structural parameters, calculate quantum chemical parameters, and predict the corrosion inhibition ability of TN derivatives at the molecular level. Specifically, the calculations were performed at the theoretical level using the 6-311++G(d,p) basis set, a highly accurate polarization–diffuse basis set that enables a good description of electron density distribution, particularly for systems containing heteroatoms such as N and O [6]. The computational procedure included geometry optimization of the molecular structures in their ground states, stability confirmation through vibrational frequency analysis, with no imaginary frequencies, and calculation of important electronic parameters related to corrosion inhibition ability. Quantities such as the frontier molecular orbital energies (E_{HOMO} and E_{LUMO}), energy gap (ΔE), hardness (η), softness (S), fraction of electrons transferred (ΔN), and atomic charges at selected active sites were used as molecular descriptors to evaluate the electronic interaction tendency of the inhibitor molecules with the metal surface.

In addition, the corrosion inhibition efficiency was estimated based on the ionization energy of TN derivatives determined according to the following equations [7]:

$$IE_{dx} \% = \frac{IE_{\text{TN}} - IE_{\text{X-TN}}}{IE_{\text{TN}}} \times 100 \quad (1)$$

$$H_{dx} \% = \frac{IE_{dx} \% \times H_{\text{tn}} \%}{100} \quad (2)$$

$$H_{\text{it}} \% = H_{dx} \% + H_{\text{tn}} \% \quad (3)$$

Here, $IE_{dx}\%$, $H_{\text{it}}\%$, $H_{\text{tn}}\%$ and $H_{dx}\%$ denote the relative change in the ionization energy of the X–TN derivative compared with TN, the corrosion inhibition efficiency estimated using the correlation model, the experimental corrosion inhibition efficiency of TN, and the relative change in the corrosion inhibition efficiency of the corresponding derivatives, respectively. IE_{TN} and $IE_{\text{X-TN}}$ are the ionization energies of TN and X–TN derivatives, respectively, where X represents the substituent groups.

3. Results and discussion

3.1. Structural optimization of tryptophan

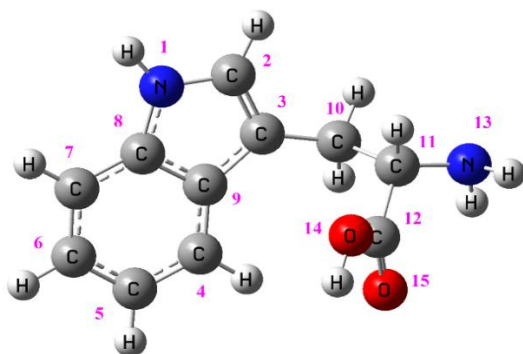


Figure 1. Optimized structure of TN at the B3LYP/6-311++G(d,p) level in the gas phase

First, the geometrical structure of tryptophan (TN) was optimized in the gas phase using the DFT method, with the B3LYP hybrid functional combined with the 6-311++G(d,p) basis set (Figure 1). Notably, the optimized structure shows the nearly perfect planarity of the indole ring system in the TN molecule. As a result, the molecule may adsorb parallel to the metal surface, maximizing the contact area and improving surface coverage efficiency. This is an important structural factor that contributes to explaining the corrosion inhibition ability of TN in the investigated environments.

3.2. Effect of OH group position on the corrosion inhibition ability of tryptophan

Previous studies have shown that polar functional groups, particularly hydroxyl groups (–OH), have a significant influence on the corrosion inhibition efficiency of organic compounds by regulating electron density and the ability to form bonds with metal surfaces [8, 9]. Therefore, in this study, the effect of the –OH group on the corrosion inhibition ability of TN was systematically investigated by replacing H atoms at different positions on the molecular framework.

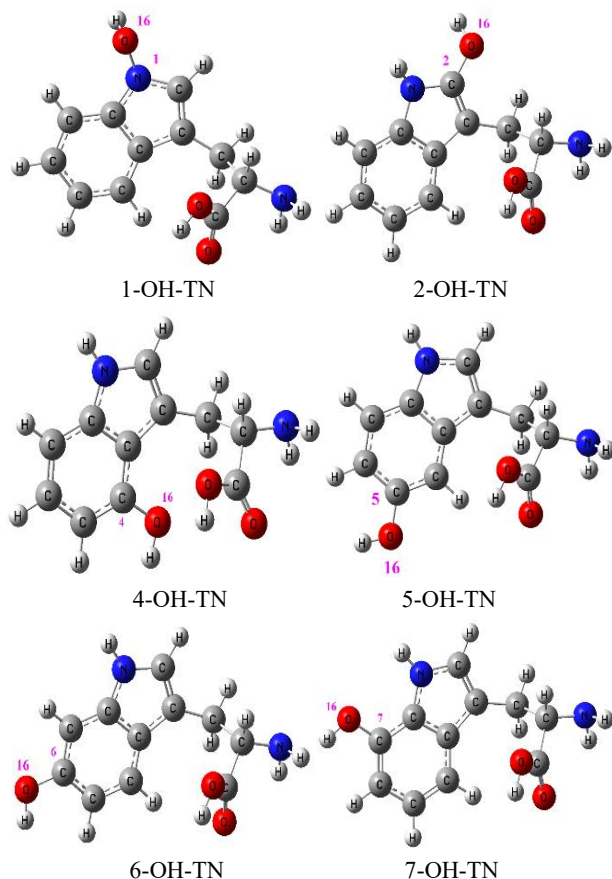


Figure 2. Optimized structures of OH-TN derivatives

When these substitutions were performed, six corresponding hydroxyl derivatives were constructed, including 1-OH-TN, 2-OH-TN, 4-OH-TN, 5-OH-TN, 6-OH-TN, and 7-OH-TN. All geometrical structures of these derivatives were fully optimized in the gas phase at the B3LYP/6-311++G(d,p) theoretical level and are presented in Figure 2.

Table 1. Structural parameters of TN and OH-TN derivatives

Compounds	TN	1-OH-TN	2-OH-TN	4-OH-TN	5-OH-TN	6-OH-TN	7-OH-TN
Bond length (Å)							
N1-C8	1.38	1.38	1.39	1.38	1.38	1.38	1.38
C8-C7	1.40	1.40	1.39	1.40	1.39	1.40	1.40
C7-C6	1.39	1.39	1.39	1.38	1.39	1.39	1.39
C6-C5	1.41	1.41	1.41	1.41	1.41	1.41	1.41
C5-C4	1.39	1.39	1.39	1.39	1.39	1.39	1.38
C4-C9	1.41	1.41	1.40	1.41	1.40	1.40	1.41
C9-C8	1.42	1.42	1.42	1.42	1.42	1.42	1.42
C9-C3	1.44	1.45	1.45	1.44	1.44	1.45	1.44
C3-C2	1.37	1.37	1.37	1.37	1.37	1.37	1.37
C2-N1	1.38	1.38	1.39	1.38	1.38	1.39	1.38
C3-C10	1.50	1.50	1.50	1.50	1.50	1.50	1.50
C10-C11	1.55	1.55	1.55	1.56	1.55	1.55	1.55
C11-C12	1.53	1.53	1.53	1.53	1.53	1.53	1.53
C12-O14	1.35	1.35	1.35	1.35	1.35	1.35	1.35
C12-O15	1.21	1.21	1.21	1.21	1.21	1.21	1.21
C11-N13	1.46	1.46	1.46	1.46	1.46	1.46	1.46
N1-O16		1.39					
C2-O16			1.36				
C4-O16				1.37			
C5-O16					1.38		
C6-O16						1.37	
C7-O16							1.37
Bond angle (°)							
N1-C8-C7	130.43	130.86	130.12	130.06	130.78	129.98	129.70
C8-C7-C6	117.52	117.07	117.55	117.03	117.87	117.12	117.96
C7-C6-C5	121.13	121.24	120.97	121.48	120.91	121.36	120.53
C6-C5-C4	121.19	121.26	121.23	120.80	121.38	120.93	121.76
C5-C4-C9	119.06	119.08	119.04	119.69	118.64	119.41	118.53
C4-C9-C8	118.70	118.31	118.67	117.85	119.29	118.29	119.03
C9-C8-C7	122.39	123.01	122.53	123.15	121.91	122.89	122.18
C9-C8-N1	107.17	106.12	107.34	106.78	107.31	107.13	108.11
C8-N1-C2	109.18	110.42	108.04	109.40	108.97	109.28	108.67
N1-C2-C3	110.12	109.16	111.30	110.15	110.28	109.99	110.15
C2-C3-C10	125.94	125.88	125.83	125.15	125.79	126.02	125.87
C3-C10-C11	115.85	115.68	115.67	116.55	115.98	115.78	115.90
C10-C11-C12	110.15	110.14	109.88	111.47	110.13	110.20	110.13
C11-C12-O14	112.86	112.85	112.90	112.30	112.88	112.88	112.84
C11-C12-O15	124.36	124.30	124.40	125.00	124.33	124.38	124.37
C10-C11-N13	108.85	108.80	108.89	108.64	108.80	108.88	108.83

The characteristic structural parameters, including bond lengths and bond angles of the OH-TN derivatives, are summarized in Table 1. In general, these values vary only slightly compared with the parent TN molecule, indicating that the attachment of the –OH group does not significantly alter the basic structural framework of the molecule. However, notable differences are observed in the dihedral angles related to the –OH group. Specifically, characteristic dihedral angles such as C3–C2–N1–O16 for 1-OH-TN, C9–C3–C2–O16 for 2-OH-TN, C6–C5–C4–

O16 for 4-OH-TN, C5–C6–C7–O16 for 5-OH-TN, C8–C7–C6–O16 for 6-OH-TN, and C9–C4–C5–O16 for 7-OH-TN are 165.75°, 176.67°, 179.97°, 179.98°, 179.96°, and 179.79°, respectively.

These results indicate that, while the –OH group in 1-OH-TN and 2-OH-TN deviates considerably from the plane of the indole ring system, in the remaining derivatives, namely 4-OH-TN, 5-OH-TN, 6-OH-TN, and 7-OH-TN, the –OH group is nearly coplanar with the aromatic ring system. This coplanarity is important from the viewpoint of surface chemistry because it enhances π conjugation and facilitates parallel adsorption of the molecule on the metal surface. Consequently, these derivatives may form a more uniform and stable protective film on the metal surface in corrosive media, thereby improving corrosion inhibition efficiency compared with structures in which the –OH group deviates from the molecular plane.

Atomic charges were determined using charge density analysis, and the obtained results are presented in Table 2. The analysis of atomic charges in Table 2 shows that hydroxyl substitution at different positions on the tryptophan framework changes the electron density distribution in the molecule, mainly at the carbon atom bearing the substituent and neighboring atoms.

Table 2. Atomic charges of OH-TN derivatives

Atoms	TN	1-OH-TN	2-OH-TN	4-OH-TN	5-OH-TN	6-OH-TN	7-OH-TN
N1	0.19	-0.20	0.16	0.20	0.19	0.19	0.16
C2	0.21	0.45	-0.15	0.33	0.24	0.23	0.31
C3	0.59	0.56	1.05	0.89	0.72	0.67	0.64
C4	-0.29	-0.39	-0.30	-0.64	-0.51	-0.31	-0.49
C5	-0.39	-0.46	-0.37	-0.47	-0.81	-0.14	-0.30
C6	0.00	0.02	-0.05	0.09	0.36	-0.39	0.23
C7	-0.24	-0.33	-0.25	-0.34	-0.27	-0.26	-0.61
C8	-0.17	-0.13	-0.23	-0.17	-0.44	-0.05	-0.24
C9	0.50	0.58	0.58	0.50	0.84	0.46	0.75
C10	-0.01	-0.04	-0.02	-0.02	0.05	-0.02	-0.07
C11	-0.33	-0.27	-0.32	-0.41	-0.33	-0.33	-0.32
C12	-0.29	-0.30	-0.28	-0.18	-0.29	-0.30	-0.29
N13	0.26	0.26	0.26	0.23	0.26	0.26	0.26
O14	0.20	0.20	0.20	0.17	0.20	0.20	0.20
O15	-0.23	-0.24	-0.24	-0.25	-0.23	-0.23	-0.23
O16		0.28	-0.03	0.07	0.03	0.02	0.01

Quantum chemical parameters play a key role in explaining and predicting the corrosion inhibition ability of organic compounds through electronic interactions with metal surfaces. Among these parameters, the energy of the HOMO, E_{HOMO} is an important parameter reflecting the electron-donating tendency of a molecule. A higher, less negative E_{HOMO} value indicates stronger electron-donating ability, thereby increasing the possibility of coordination bond formation between the inhibitor molecule and the vacant orbitals of the metal, contributing to enhanced corrosion inhibition efficiency.

The results presented in Table 3 show that the E_{HOMO} of

TN is -5.75 eV. When hydroxyl groups ($-\text{OH}$) are substituted at different positions on the molecular framework, the E_{HOMO} values tend to increase, ranging from -5.82 to -5.49 eV. Specifically, the E_{HOMO} values are -5.82 , -5.68 , -5.49 , -5.61 , -5.49 , and -5.57 eV for 1-OH-TN, 2-OH-TN, 4-OH-TN, 5-OH-TN, 6-OH-TN, and 7-OH-TN, respectively. Notably, the 4-OH-TN and 6-OH-TN derivatives have the highest E_{HOMO} values, indicating superior electron-donating ability compared with the other molecules.

Table 3. Quantum chemical parameters of TN derivatives containing OH groups

Compounds	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	η (eV)	S (eV^{-1})	ΔN
TN	-5.75	-0.70	5.05	2.52	0.40	0.32
1-OH-TN	-5.82	-0.86	4.96	2.48	0.40	0.30
2-OH-TN	-5.68	-0.75	4.93	2.47	0.41	0.32
4-OH-TN	-5.49	-0.50	4.99	2.50	0.40	0.37
5-OH-TN	-5.61	-0.77	4.83	2.42	0.41	0.34
6-OH-TN	-5.49	-0.64	4.85	2.42	0.41	0.37
7-OH-TN	-5.57	-0.52	5.05	2.53	0.40	0.35

From the E_{HOMO} values, the corrosion inhibition efficiencies of OH-TN derivatives were determined using Equations (1), (2), and (3), and the results are summarized in Table 4. The parent compound TN was reported to have a corrosion inhibition efficiency for steel in 1.0 M HCl solution of 89.56%, as determined by the electrochemical polarization curve method [10]. This experimental value was used as the reference basis for calculating the inhibition efficiencies of the corresponding hydroxyl derivatives.

Table 4. Estimated corrosion inhibition efficiency of TN derivatives containing OH groups for steel

Compounds	IE	IE _{dx} %	H _{dx} %	H _{in} %	H _{it} %
TN	5.75	0.00	0.00	89.56	89.56
1-OH-TN	5.82	-1.22	-1.09		88.47
2-OH-TN	5.68	1.22	1.09		90.65
4-OH-TN	5.49	4.52	4.05		93.61
5-OH-TN	5.61	2.43	2.18	91.28	91.74
6-OH-TN	5.49	4.52	4.05		93.61
7-OH-TN	5.57	3.13	2.80		92.36

Specifically, the inhibition efficiencies of 1-OH-TN, 2-OH-TN, 4-OH-TN, 5-OH-TN, 6-OH-TN, and 7-OH-TN are 88.47%, 90.65%, 93.61%, 91.74%, 93.61%, and 92.36%, respectively. In general, most OH-TN derivatives exhibit higher inhibition efficiency than the parent TN compound, indicating the positive role of the hydroxyl group in enhancing metal protection. Notably, the 4-OH-TN and 6-OH-TN derivatives show the highest inhibition efficiency of 93.61%, suggesting that these compounds have superior potential for inhibiting steel corrosion in acidic media. This result is also consistent with the previous analyses based on quantum chemical parameters, further supporting the relationship between electronic structure and corrosion inhibition efficiency.

In addition, the agreement between the theoretical calculation results and experimental data is clearly

demonstrated. Specifically, for the 5-OH-TN derivative, the calculated inhibition efficiency is 91.74%, which is very close to the experimental value of 91.28% (± 0.94). This small difference indicates that the applied models and Equations (1), (2), and (3) can reasonably reflect the trend in corrosion inhibition efficiency for the investigated compound system, thereby supporting the screening and design of potential inhibitors.

Furthermore, molecular reactivity is related to the HOMO–LUMO energy gap (ΔE). A smaller ΔE is commonly associated with greater molecular reactivity and polarizability and may therefore favor interaction with the metal surface. The ΔE value is determined according to Equation (4).

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} \quad (4)$$

The data in Table 3 show that 5-OH-TN and 6-OH-TN have the two smallest ΔE values, 4.83 and 4.85 eV, respectively, suggesting a greater tendency to interact with the metal surface than the other investigated derivatives.

In addition, the hardness, η , and softness, S , parameters were also used to evaluate the reactivity and interaction ability of the molecules. Theoretically, an effective inhibitor generally has low hardness and high softness, meaning that its electron cloud can be easily deformed to interact with the metal surface. These quantities are calculated using Equations (5) and (6).

$$\eta = \frac{IE - EA}{2} = \frac{E_{\text{LUMO}} - E_{\text{HOMO}}}{2} \quad (5)$$

$$S = \frac{1}{\eta} \quad (6)$$

The results in Table 3 show that 5-OH-TN and 6-OH-TN have the lowest hardness values, $\eta \approx 2.42$ eV, and the highest softness values, $S \approx 0.41$ eV^{-1} , among the investigated compounds, indicating their stronger electronic interaction ability with the metal surface compared with the other derivatives.

The fraction of electrons transferred (ΔN) is estimated using Equation (7) as a conceptual DFT descriptor of the electron-donation tendency between the inhibitor molecule and the metal surface, where χ and η are the absolute electronegativity and hardness of the inhibitor, respectively, and Φ is the work function of the metal surface:

$$\Delta N = \frac{\Phi - \chi_{\text{inh}}}{2(\eta_{\text{Fe}} + \eta_{\text{inh}})} \quad (7)$$

In this study, Φ of the Fe(110) surface is taken as 4.82 eV [11]. The calculated ΔN values for the OH-TN derivatives range from 0.30 to 0.37. According to Lukovits et al. [12], positive ΔN values below 3.6 are generally associated with a tendency for electron donation from the inhibitor to the metal surface. All investigated OH-TN derivatives satisfy this criterion, suggesting that electron donation to the Fe(110) surface is energetically favorable within the conceptual DFT framework. Compared with TN ($\Delta N = 0.32$), 4-OH-TN, 5-OH-TN, 6-OH-TN, and 7-OH-TN exhibit higher ΔN values, whereas 2-OH-TN shows a similar value and 1-OH-TN a slightly lower one. These

results indicate that the influence of hydroxyl substitution on the predicted electron-transfer tendency strongly depends on the substitution position.

Based on the analyzed quantum chemical parameters, 6-OH-TN exhibits a favorable overall combination of electronic descriptors, including one of the highest E_{HOMO} values, low ΔE and hardness η , together with high softness S and ΔN . Although 5-OH-TN shows a slightly smaller ΔE value, 6-OH-TN displays a more balanced combination of descriptors associated with corrosion inhibition potential. These features indicate that 6-OH-TN is the most promising candidate for the research and development of effective metal corrosion inhibitors.

3.3. Effect of electron-donating substituents on the steel corrosion inhibition ability of TN

In addition to the hydroxyl group ($-\text{OH}$), other electron-donating substituents are also expected to significantly affect the electronic characteristics and thus influence the corrosion inhibition ability of the TN framework. On this basis, the study further investigated the effects of several typical electron-donating groups, such as $-\text{NH}_2$, $-\text{OCH}_3$, and $-\text{CH}_3$, through characteristic quantum chemical parameters (Figure 3).

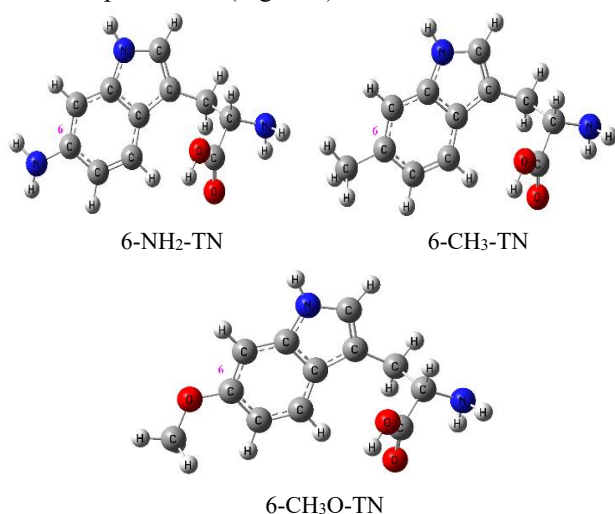


Figure 3. Optimized structures of TN derivatives containing electron-donating groups

Table 5. Quantum chemical parameters and estimated inhibition efficiencies of TN derivatives containing electron-donating groups

Compounds	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	η (eV)	S (eV ⁻¹)	ΔN	$H_{\text{it}}\%$
6-NH ₂ -TN	-5.16	-0.50	4.66	2.33	0.43	0.43	98.75
6-CH ₃ -TN	-5.63	-0.59	5.04	2.52	0.40	0.34	91.43
6-OCH ₃ -TN	-5.38	-0.61	4.77	2.38	0.42	0.38	95.32

The results presented in Table 5 show clear variations in electronic parameters upon substitution with different functional groups. Notably, the 6-NH₂-TN derivative exhibits the most favorable characteristics among the investigated compounds, with the highest E_{HOMO} value of -5.16 eV, indicating strong electron-donating ability. At the same time, this compound also has the smallest

energy gap, ΔE , of 4.66 eV, suggesting greater polarizability/reactivity. In addition, the global hardness η , of 6-NH₂-TN reaches the lowest value of 2.33 eV, while the softness, S , reaches the highest value of 0.43 eV⁻¹, indicating that the electron cloud of the molecule is easily deformable and favorable for adsorption and electron exchange with the metal surface. This molecule also has the highest ΔN value of 0.43 , reflecting the tendency of the inhibitor molecule to donate electrons to the Fe(110) surface. As a result, the adsorption of the inhibitor on the Fe surface can be enhanced.

When this compound is compared with the 6-OH-TN derivative, which has been identified as an effective inhibitor, 6-NH₂-TN is still superior in all important quantum chemical parameters. This is supported by the calculated inhibition efficiency, in which 6-NH₂-TN reaches a value of up to 98.75% , significantly higher than that of 6-OH-TN. This result indicates that the $-\text{NH}_2$ group has stronger electron-donating ability, contributing to an increase in electron density on the molecule and enhancing adsorption interactions on the metal surface, thereby improving corrosion inhibition efficiency.

4. Conclusion

The effect of electron-donating substituents on the steel corrosion inhibition ability of TN derivatives was investigated using DFT at the B3LYP/6-311++G(d,p) level. Characteristic quantum chemical parameters, including the energy of the HOMO (E_{HOMO}), the energy gap (ΔE), hardness (η), softness (S), and fraction of electrons transferred (ΔN), were used as quantitative criteria to analyze the tendency of electronic interactions between the inhibitor molecule and the metal surface.

The results show that electron-donating substitution generally produces favorable changes in the quantum chemical descriptors of TN derivatives; however, the magnitude and direction of these changes depend on both the substituent type and substitution position. Most of the investigated derivatives exhibit higher estimated corrosion inhibition efficiencies than the parent TN compound.

Among the investigated compounds, 6-NH₂-TN exhibits the most favorable combination of computed electronic descriptors, including strong electron-donating ability, a relatively small energy gap, low hardness, high softness, and a high ΔN value. These characteristics suggest an enhanced electronic interaction tendency with the Fe surface and result in the highest estimated inhibition efficiency among the investigated derivatives. The close agreement between the estimated and experimental inhibition efficiencies for 5-OH-TN provides support for the applicability of the correlation approach, although further experimental validation is required for the newly proposed derivatives.

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APPENDIX

Table S1. Optimized structures of TN and TN derivatives at the B3LYP/6-311++G(d,p) level

TN			C ₁₁ H ₁₂ N ₂ O ₂
0 1			
O	1.64498300	-0.86499500	1.83848700
O	2.26799000	-1.91976700	-0.04587800
N	-1.81526900	2.03261400	0.49388200
N	3.80004500	0.51909200	-0.59691400
C	0.02448200	1.11745100	-0.44044200
C	1.41935900	0.96482000	-0.97488200
C	-1.02151100	0.12230500	-0.39944700
C	2.48697500	0.49362800	0.04652600
C	-2.16030900	0.73197700	0.19223000
C	-0.50766200	2.25690300	0.10684300
C	-1.11274200	-1.21735100	-0.81561600

C	-3.36412200	0.04768100	0.37752500
C	-2.30709400	-1.89929500	-0.63466700
C	-3.42191600	-1.27386800	-0.04257500
C	2.13053700	-0.89457200	0.57827600
H	1.78393500	1.91912800	-1.36265300
H	1.42454800	0.26280200	-1.81579400
H	2.49860500	1.18991200	0.88715000
H	-0.05444300	3.22670100	0.24698700
H	-2.42350900	2.71831900	0.90807000
H	-0.26109300	-1.71609700	-1.26400800
H	-4.22395700	0.52923300	0.83061400
H	-4.34135400	-1.83375200	0.08552300
H	3.85581400	-0.21463100	-1.29842000
H	4.53803700	0.34126400	0.07717100
H	1.39746300	-1.77241600	2.07644600
H	-2.38724600	-2.93238000	-0.95336400
1-OH-TN			C ₁₁ H ₁₂ N ₂ O ₃
0 1			
O	-1.89748000	0.53872200	1.93493300
O	-2.74027200	1.69537900	0.20163500
N	1.93033800	-1.56733300	0.07137700
N	-3.91053900	-0.87731500	-0.59318900
C	-0.08607000	-0.87097900	-0.62453000
C	-1.51216700	-0.88583900	-1.09626100
C	0.79304800	0.27069000	-0.50616700
C	-2.58725200	-0.71680600	0.00839700
C	2.04595000	-0.19808900	-0.02585300
C	0.64247100	-1.96516200	-0.23275300
C	0.64969500	1.64456100	-0.76332000
C	3.12355300	0.64789600	0.23792500
C	1.71957000	2.49256600	-0.51460500
C	2.94000200	2.00131100	-0.01121500
C	-2.42624200	0.63893900	0.69661600
H	-1.74073100	-1.83391600	-1.58850500
H	-1.66868900	-0.09967300	-1.84262800
H	-2.44831200	-1.49981400	0.75606800
H	0.37236500	-3.00727700	-0.16458400
H	-0.28816000	2.04126100	-1.13481600
H	4.05721400	0.26345000	0.62973400
H	3.75147800	2.69272100	0.18530000
H	-4.11872600	-0.08122300	-1.19022100
H	-4.63206900	-0.91060600	0.12015000
H	-1.78440600	1.43907500	2.27839200
H	1.61499300	3.55458900	-0.70493300
O	2.82526100	-2.36959200	0.76407000
H	3.43104700	-2.71665000	0.09422800
2-OH-TN			C ₁₁ H ₁₂ N ₂ O ₃
0 1			
O	1.65127900	-0.95888900	1.88566700
O	2.24487200	-2.18935700	0.10136400
N	-1.79301700	1.84156100	0.38050300
N	3.79641800	0.15643900	-0.70648200
C	0.03672800	0.81731500	-0.49696800
C	1.41502400	0.62363000	-1.05376300
C	-1.04641100	-0.13986900	-0.41819100
C	2.50392500	0.21882000	-0.02633000
C	-2.16700800	0.52396800	0.14604700
C	-0.46313100	1.98204200	0.01462200
C	-1.17767300	-1.48681600	-0.78724500
C	-3.38509700	-0.11512100	0.36256000
C	-2.39157800	-2.12966400	-0.57396700

C	-3.48263400	-1.45475400	-0.00085100
C	2.13014300	-1.10951600	0.63108100
H	1.77162600	1.54981200	-1.51012900
H	1.39500900	-0.13560900	-1.84281100
H	2.55385500	0.98628500	0.74792700
H	-2.26291000	2.46778300	1.01516900
H	-0.34169400	-2.02547700	-1.21866200
H	-4.22971800	0.41003700	0.79527700
H	-4.41581300	-1.98308500	0.15714800
H	3.82330500	-0.64943600	-1.32563500
H	4.55256400	0.04353700	-0.03873600
H	1.39179400	-1.83765500	2.20463300
H	-2.49976300	-3.17185800	-0.85224900
O	0.18841700	3.16094100	0.21384100
H	-0.27233100	3.87790000	-0.23902700
4-OH-TN		C ₁₁ H ₁₂ N ₂ O ₃	
0 1			
O	1.43641100	-0.59089500	1.80377600
O	2.84854800	-1.72039300	0.46971900
N	-1.79728300	2.21162900	0.34311500
N	3.81041600	0.74488700	-0.59378700
C	0.00891900	1.14047700	-0.48721100
C	1.40021500	0.90647800	-1.00726900
C	-1.07160100	0.19689500	-0.32714600
C	2.50708200	0.65181700	0.05709300
C	-2.18764800	0.89962600	0.19441000
C	-0.48615400	2.35057900	-0.07298300
C	-1.22094700	-1.17902800	-0.57985300
C	-3.41715200	0.28833300	0.46965300
C	-2.43312400	-1.79937200	-0.31272100
C	-3.51830700	-1.06790600	0.20803500
C	2.30213600	-0.68696400	0.76866600
H	1.74013800	1.78994500	-1.55320300
H	1.40188000	0.07317100	-1.71346100
H	2.43822000	1.44006200	0.81111500
H	-0.00258600	3.31528800	-0.04688500
H	-2.38324200	2.95824800	0.67605700
H	-4.25403000	0.84945900	0.86846700
H	-4.45106500	-1.58395600	0.40393600
H	3.94081700	-0.05187100	-1.21187200
H	4.55558400	0.69246600	0.09395000
H	1.32127700	-1.48225400	2.16723800
H	-2.54719600	-2.86105500	-0.51067500
O	-0.13581600	-1.84630900	-1.08595300
H	-0.34538900	-2.77995000	-1.19433800
7-OH-TN		C ₁₁ H ₁₂ N ₂ O ₃	
0 1			
O	1.89526400	-0.77972500	1.88266900
O	2.68686700	-1.84751300	0.07025600
N	-1.61499300	1.92120700	0.29398700
N	4.11272900	0.65320100	-0.47287300
C	0.30926800	1.06613900	-0.51959000
C	1.73509900	0.96738800	-0.97991300
C	-0.68737600	0.02114600	-0.50347600
C	2.77173800	0.57589000	0.10538800
C	-1.87231100	0.59998100	0.01136100
C	-0.30303600	2.19530800	-0.03266600
C	-0.69831500	-1.33588800	-0.88362200
C	-3.05500700	-0.12983500	0.15628800
C	-1.87321800	-2.05392300	-0.73822600
C	-3.04630500	-1.46264200	-0.22174100
C	2.45787300	-0.81553100	0.65512400
H	2.07311900	1.92788500	-1.37638000
H	1.81574000	0.24474600	-1.79922100
H	2.70567600	1.29176200	0.92686400
H	0.09841400	3.18847400	0.10107200
H	-2.28748400	2.57465500	0.65830800
H	0.19239800	-1.81317400	-1.27354300
H	-3.95074800	-2.05529800	-0.12153900
H	4.24034400	-0.09364500	-1.15075800
H	4.82338700	0.52901800	0.24142600
H	1.67946400	-1.69254900	2.13046800
H	-1.90309400	-3.09868600	-1.02560700
O	-4.14505600	0.53594900	0.66452400
H	-4.89843800	-0.06193900	0.70797200
5-OH-TN		C ₁₁ H ₁₂ N ₂ O ₃	
0 1			
O	-2.69562600	-2.64427100	-0.59036200
O	1.71735400	-0.76838800	1.90662800
O	2.16737500	-2.09183400	0.14654700
N	-1.21651200	2.56830500	0.34537800
N	4.01827200	0.01498900	-0.67466900
C	0.39901000	1.24408800	-0.51255000
C	1.72609700	0.79666000	-1.05342100
C	-0.79889500	0.45789500	-0.33941300
C	2.73934500	0.25882300	-0.00876600
C	-1.79140900	1.31945200	0.19911100
C	0.09098700	2.51357800	-0.08930900
C	-1.12214900	-0.88397000	-0.60079300
C	-3.08165600	0.87303800	0.47819900
C	-2.40717800	-1.32408900	-0.32369500
C	-3.38019800	-0.45698200	0.21241300
C	2.18668100	-0.99920900	0.66074800
H	2.23172300	1.62831100	-1.55022100
H	1.58069400	0.02070600	-1.81299800
H	2.88668800	1.02035500	0.75943000
H	0.71147200	3.39699300	-0.07086600
H	-1.68208700	3.39259400	0.68432500
H	-0.39816000	-1.58129700	-1.00436900
H	-3.83668400	1.53457300	0.88819800
H	-4.37712300	-0.83464800	0.41910600
H	3.93420300	-0.78112000	-1.30147600
H	4.73950600	-0.21722400	0.00110700
H	1.33736800	-1.59980100	2.23176200
H	-3.61655600	-2.82225900	-0.37660500
6-OH-TN		C ₁₁ H ₁₂ N ₂ O ₃	
0 1			
O	1.87861200	-1.00039200	1.85382100
O	2.26817000	-2.10758600	-0.06260200
N	-1.18430500	2.35204800	0.49555500
N	4.17264200	0.07410300	-0.58942100
C	0.52084200	1.20563000	-0.43951100
C	1.88356300	0.86522000	-0.97013200
C	-0.65262900	0.36124900	-0.40951800
C	2.86785400	0.23990600	0.05109600
C	-1.70112900	1.11532200	0.18263900
C	0.14757600	2.40151700	0.11402700
C	-0.93199100	-0.94630400	-0.83446500
C	-2.99069200	0.61044700	0.36153600
C	-2.20914400	-1.45964200	-0.66372500
C	-3.22750700	-0.68647100	-0.06990700
C	2.31249800	-1.08347300	0.57732400

H	2.37966200	1.76284800	-1.34700800
H	1.79539200	0.17672500	-1.81770300
H	2.98014600	0.92371800	0.89435900
H	0.72590000	3.30040800	0.26417800
H	-1.69706300	3.11099200	0.91111900
H	-0.16098400	-1.56131700	-1.28357200
H	-3.78962300	1.18719700	0.81162500
H	4.12221600	-0.65519800	-1.29583500
H	4.87539700	-0.21227500	0.08491200
H	1.50480900	-1.86368400	2.09101200
H	-2.43289100	-2.47113000	-0.99005700
O	-4.49641800	-1.18471300	0.10641200
H	-4.53967900	-2.08023600	-0.24319600
6-NH₂-TN		C₁₁H₁₃N₃O₂	
0 1			
O	1.84281600	-1.01177900	1.83736500
O	2.29468900	-2.11963900	-0.06506800
N	-1.16995500	2.35993600	0.48728900
N	4.18656300	0.06816900	-0.56967200
C	0.53656200	1.20953600	-0.43876200
C	1.90108700	0.86544900	-0.96202600
C	-0.63807900	0.36729200	-0.41037800
C	2.87722700	0.23106300	0.06240200
C	-1.68656500	1.12186500	0.17619000
C	0.16464600	2.40766800	0.11124000
C	-0.92368000	-0.94162200	-0.83189600
C	-2.97790900	0.61764500	0.35090600
C	-2.19908000	-1.45203400	-0.66165300
C	-3.23437200	-0.68506500	-0.07312100
C	2.31510500	-1.09467700	0.57474400
H	2.40378100	1.76272700	-1.33105000
H	1.81597800	0.18115900	-1.81344800
H	2.98328500	0.90917800	0.91110800
H	0.74380900	3.30573800	0.26266000
H	-1.68040300	3.11786500	0.90714300
H	-0.15411400	-1.55976900	-1.27999200
H	-3.76044600	1.21577500	0.80716500
H	4.13902800	-0.65662700	-1.28099100
H	4.88248000	-0.22687600	0.10810000
H	1.45784400	-1.87368000	2.06135000
H	-2.41758800	-2.46659400	-0.97908400
N	-4.49421100	-1.27096900	0.13243300
H	-5.26052800	-0.61846900	0.21693700
H	-4.71959700	-2.02174400	-0.50450200
6-CH₃-TN		C₁₂H₁₄N₂O₂	
0 1			
O	1.84774500	-1.02213900	1.83414500
O	2.30957600	-2.13386800	-0.06367500
N	-1.14088100	2.36950700	0.49881300
N	4.19856500	0.05275200	-0.57300600
C	0.55277900	1.20556800	-0.43387000
C	1.91430100	0.85431100	-0.96060000
C	-0.62913200	0.37570000	-0.41165200
C	2.89105600	0.21727800	0.06163800
C	-1.66957000	1.13729800	0.17812000

C	0.18994700	2.40494800	0.12372600
C	-0.92356000	-0.92993400	-0.84228000
C	-2.96465100	0.63740100	0.34682500
C	-2.20720400	-1.42288900	-0.67576700
C	-3.23872800	-0.65577500	-0.08313700
C	2.32684300	-1.10778100	0.57391300
H	2.41990300	1.74856800	-1.33302500
H	1.82279200	0.16928600	-1.81059200
H	3.00001000	0.89443200	0.91083300
H	0.77886400	3.29622900	0.27923300
H	-1.64624800	3.13254500	0.91599000
H	-0.15699000	-1.55065500	-1.29219800
H	-3.74210100	1.24364500	0.80124600
H	4.14892700	-0.67177000	-1.28446000
H	4.89565700	-0.24309200	0.10317700
H	1.46471200	-1.88476900	2.05863200
H	-2.43429600	-2.43058900	-1.00918800
C	-4.61987700	-1.24770100	0.07098200
H	-4.59754000	-2.15465000	0.68379400
H	-5.30605000	-0.54217800	0.54448700
H	-5.04321900	-1.52530000	-0.89973200
6-CH₃O-TN		C₁₂H₁₄N₂O₃	
0 1			
O	2.06484600	-1.09523700	1.86165600
O	2.30011900	-2.29436500	-0.02441200
N	-0.49366400	2.63176700	0.46003700
N	4.47464000	-0.40719300	-0.61663500
C	1.02044700	1.23156100	-0.46027200
C	2.31480200	0.68994300	-0.99453600
C	-0.26003200	0.56172800	-0.39590200
C	3.21315900	-0.04799400	0.03128900
C	-1.18446600	1.47171700	0.18569000
C	0.82626800	2.48174900	0.06369500
C	-0.72869700	-0.70082400	-0.78008300
C	-2.52591200	1.15684100	0.38882900
C	-2.06498800	-1.03132800	-0.58588000
C	-2.95814000	-0.10718600	-0.00349600
C	2.48358100	-1.26969600	0.58928700
H	2.92902100	1.50010200	-1.39494900
H	2.12016000	0.00387600	-1.82622700
H	3.42914800	0.62968000	0.85921900
H	1.52794500	3.29328400	0.18316100
H	-0.88855200	3.46664800	0.85806800
H	-0.05867200	-1.43042100	-1.22006800
H	-3.23117400	1.85061800	0.83042300
H	4.31418200	-1.13589000	-1.30709600
H	5.13715100	-0.77730800	0.05771500
H	1.57395900	-1.89174900	2.11816300
H	-2.41188500	-2.00979300	-0.88810700
O	-4.28599700	-0.36908900	0.21767800
C	-4.80947200	-1.62896700	-0.17379600
H	-5.86649700	-1.60527900	0.08792600
H	-4.70855900	-1.78952400	-1.25291700
H	-4.32410300	-2.45200700	0.36255500