



## A Computational Study of Quinoline Derivatives as Corrosion Inhibitors for Mild Steel in Acidic Medium

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**ABSTRACT:** The corrosion inhibition efficiency of three quinoline derivatives namely; ethyl 2-(((8-hydroxyquinolin-5-yl)methyl)amino)acetate (QN1), 5-((benzylamino)methyl)quinolin-8-ol (QN2) and 5-(azidomethyl)quinolin-8-ol (QN3) on the mild steel in 1 M HCl was studied using density functional theory (DFT) calculations and quantitative structural activity relationship (QSAR) approach. The experimental inhibition efficiency were discussed in relation with molecular descriptors such as such as  $E_{HOMO}$  (energy of the highest occupied molecular orbital),  $E_{LUMO}$  (energy of the lowest unoccupied molecular orbital), band gap (BG), dipole moment (DM), chemical hardness ( $\eta$ ), softness ( $\sigma$ ), electronegativity ( $\chi$ ), electrophilicity ( $\omega$ ), global nucleophilicity ( $\epsilon$ ), electrons transferred from inhibitors to metal surface ( $\Delta N$ ), initial molecule-metal interaction energy ( $\Delta\psi$ ), the energy change during electronic back-donation process ( $\Delta E_{b-d}$ ), Molecular weight (MW), and Volume (V). The result showed that  $E_{HOMO}$ ,  $\sigma$ ,  $\omega$ ,  $\Delta N$ ,  $\Delta E_{b-d}$  and  $\Delta\psi$  increases as the percentage inhibition efficiency (%IE) increases.  $E_{LUMO}$ , BG,  $\eta$ , DM, and  $\epsilon$  decreases with increasing % IE, while  $\chi$ , MW and V did not show any correlation with %IE. The QSAR model developed reproduced the observed corrosion inhibition efficiencies of these compounds well with a cross validation (CV.  $R^2$ ) value of 0.9994 and adjusted squared correlation coefficient ( $R^2_{adj}$ ) value of 0.9988. The results obtained in the study are in good agreement with experimental inhibition efficiency results reported earlier in literature.

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Mild steel is frequently used in various industrial applications because of its high mechanical strength, ductility, malleability and cost-effectiveness. However when it come in contact with acid during various industrial processes such as acid pickling, de-rusting, acid descaling, acid cleaning, oil well acidification, it undergoes corrosion (Khadiri *et al.*, 2016; Dohare *et al.*, 2018). Corrosion of metals causes great economic loss and can also lead to environmental pollution. The use of corrosion inhibitors, mostly heterocyclic compounds is one of the effective methods that can be used to avert the corrosion of metal in acidic solution (Khaled, 2008). This is because most of these heterocyclic compounds have atoms with lone pair of electrons (e.g., heteroatoms such as N, O, S and P). They possess  $\pi$  conjugate double bond and aromatic systems. This unique molecular structure makes it easy for them to be absorbed on the metal surface and block the active site thereby reducing corrosion. Quinoline structure (1-aza-naphthalene) is a nitrogen containing heterocycle present in many compounds exhibiting a vast range of biological activities such as antimalarial, anti-bacterial, antifungal, anthelmintic, cardiotoxic, anticonvulsant, anti-inflammatory, and analgesic activity (Rajesh, 2018). Some quinoline derivatives have also been studied as corrosion inhibitors, on

various metals and in various environments, due to  $\pi$ -electrons and nitrogen atoms in their ring (Al-Uqaily, 2015; Eldesoky and Nozha, 2017). Great advancement in computing has made quantum chemical methods a more viable tool in determining the molecular structures, electronic structure and reactivity of molecules. Computational chemist now use quantum chemical calculations to predict the corrosion inhibition performances of molecules because of the high cost of experimental methods and also because the study of the inhibition mechanisms of chemical compounds is time consuming (El-Lateef *et al.*, 2017). Quantum chemical calculation methods can be used to obtain molecular properties that might be helpful in selecting potential molecules, among a list of molecules, as possible candidates for corrosion inhibition. Moreso, quantum chemical calculation methods are now extensively utilized to help explain trends in experimental results. The conceptual density functional theory (DFT) is one of the important tool in quantum chemistry that has been accurately used to understand the reactivity and selectivity of molecules (Obot *et al.*, 2015). Lgaz *et al.*, (2016) studied experimentally three quinoline derivatives as corrosion inhibitors against mild steel in acidic medium. They reported that the studied compounds act as good corrosion inhibitors for mild steel in 1 M

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HCl. However they did not carry out the evaluation of the corrosion inhibition efficiency of the quinoline derivatives using quantum chemical calculations. Hence the aim of this work is to extend the study of Lgaz *et al.*, on the corrosion inhibition property of quinoline derivatives using DFT method to calculate molecular descriptors to gain further insight into the

factors responsible for the corrosion inhibitory properties of the studied compounds. In addition, we will correlate the calculated parameters to the experimentally observed inhibition efficiencies and establish a QSAR model from the calculated descriptors that could predict the experimental inhibition efficiencies of this class of compounds.

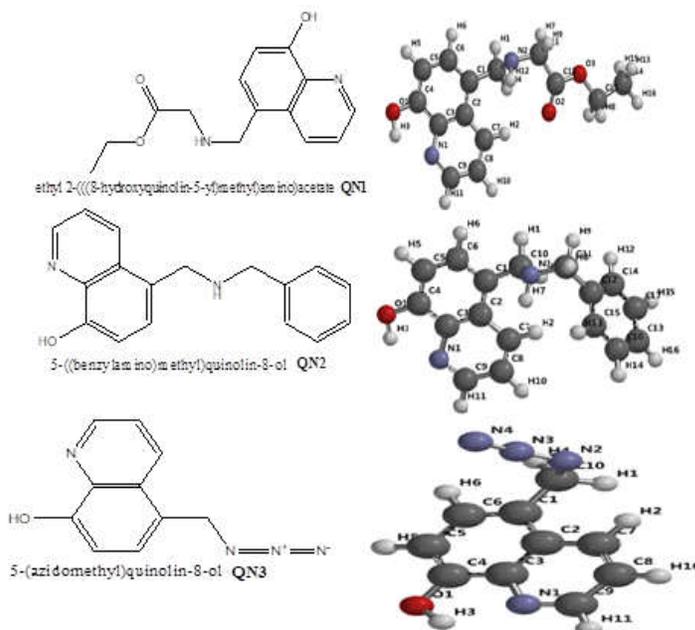


Fig 1: Chemical and Optimized Structures of the Studied Quinoline Derivative

## THEORETICAL METHODS

**Quantum Chemical Calculations:** The molecular structures of the studied quinoline derivatives (Figure1) were drawn using Symyx draw and the molecular compounds were optimized using Spartan '14 by wave function Inc. The most stable conformer was first determined for each compound by molecular mechanics (MM) using the Merck molecular force field (MMFF). DFT calculation was carried out with the three-parameter B3LYP density functionals, i.e. Becke's gradient exchange correlation (Becke, 1993) and the Lee, Yang, Parr correlation functional (Lee *et al.*, 1988). Also, the optimization were carried out using 6-31G\* as basis set in vacuum.

Many descriptors like chemical hardness ( $\eta$ ), electronegativity ( $\chi$ ), chemical potential ( $\mu$ ), global electrophilicity index ( $\omega$ ), electron affinity and ionization potential were all clarified based on  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  which were related to Koopmans' theorem (Geerlings *et al.*, 2003) using the following equations (Pauling 1960):

$$\eta = \frac{IP-EA}{2} = \frac{E_{\text{LUMO}} - E_{\text{HOMO}}}{2} \quad (1)$$

Chemical softness ( $\sigma$ ) known as a measure of the polarizability of a molecule and is mathematically defined as the multiplicative inverse of chemical hardness.

$$\sigma = \frac{1}{\eta} \quad (2)$$

Electronegativity ( $\chi$ ):

$$\chi = -\mu = \frac{IP+EA}{2} = -\frac{E_{\text{LUMO}}+E_{\text{HOMO}}}{2} \quad (3)$$

IP is ionization potential  $\approx -E_{\text{HOMO}}$  and EA is electron affinity  $\approx -E_{\text{LUMO}}$  and  $\mu$  is the chemical potential.

The electrophilicity index

$$(\omega) = \frac{\mu^2}{2\eta} \quad (4)$$

Nucleophilicity ( $\varepsilon$ ), which is the inverse of the electrophilicity is expressed as:

$$\varepsilon = \frac{1}{\omega} \quad (5)$$

When there is a close contact between an iron and an inhibitor, electrons flow from lower electronegative (inhibitor) to higher electronegative (iron), until their

chemical potentials ( $\mu$ ) or electronegativities ( $\chi$ ) become equal. The fraction of electrons transferred ( $\Delta N$ ) is given as:

$$\Delta N = \frac{\chi_{\text{Fe}} - \chi_{\text{inh}}}{2(\eta_{\text{Fe}} + \eta_{\text{inh}})} \quad (6)$$

Where  $\chi_{\text{Fe}}$  and  $\chi_{\text{inh}}$  represent the electronegativities of Fe (metal) and inhibitor respectively.  $\eta_{\text{Fe}}$  and  $\eta_{\text{inh}}$  are the chemical hardness values of Fe (metal) and inhibitor respectively. In this study, the theoretical value of  $\chi_{\text{Fe}}$  and  $\eta_{\text{Fe}}$  used to calculate the number of transferred electrons are 7 eV/mole and 0 eV/mole respectively (Parr *et al.*, 1999).

According to the charge transfer model proposed by Gomez *et al.*, (2006) for donation and back-donation of charges, an electronic back-donation process may also govern the interaction between the inhibitor molecule and the metal surface. As a result of this, if both the electron transfer to the molecule and back-donation from the molecule occurs simultaneously, the energy change is directly proportional to the hardness of the molecule (Gomez *et al.*, 2006). Hence the energy of back donation ( $\Delta E_{\text{b-d}}$ ) is expressed as:

$$(\Delta E_{\text{b-d}}) = \frac{\eta}{4} \quad (7)$$

The initial molecule-metal interaction energy ( $\Delta\psi$ ) is another significant parameter which has been calculated by Sastri and Perumareddi using equation 8 (Sastri and Perumareddi 2007)

$$\Delta\psi = \frac{(\chi_{\text{Fe}} - \chi_{\text{inh}})^2}{4(\eta_{\text{Fe}} + \eta_{\text{inh}})} \quad (8)$$

**QSAR Studies:** QSAR model was developed to predict the corrosion inhibition efficiencies of the quinoline derivatives by utilizing experimental data and molecular descriptors calculated using quantum chemical calculations. In this study, QSAR model was developed via multiple linear regression method where calculated molecular parameters served as the independent variable and the observed percentage inhibition efficiency (%IE) values reported by Lgaz *et al.*, (2016) were used as the dependent variable. In this type of analysis, the efficiency and quality of the model depends on the fitting and prediction ability. The linear equation (equation 9) proposed by Lukovits *et al.*, (2001) was used to compare the molecular parameters with the observed %IE of the organic compounds used as corrosion inhibitors.

$$\text{Predicted \%IE} = \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n \quad (9)$$

$\alpha$  and  $\beta$  are regression constants which can be obtained via regression study;  $X_1, X_2, \dots, X_n$  denotes descriptors obtained from optimization of the studied molecules.

The QSAR model validation was accomplished using statistical equations such as cross validation ( $CV.R^2$ ) and adjusted squared correlation coefficient ( $R_{\text{adj}}^2$ ).  $CV.R^2$  and  $R_{\text{adj}}^2$  were calculated using equations (10) and (11) respectively.

$$CV.R^2 = 1 - \frac{\sum(Y_{\text{obs}} - Y_{\text{cal}})^2}{\sum(Y_{\text{obs}} - \bar{Y}_{\text{obs}})^2} \quad (10)$$

$$R_{\text{adj}}^2 = \frac{(N-1) \times R^2 - P}{N-1-P} \quad (11)$$

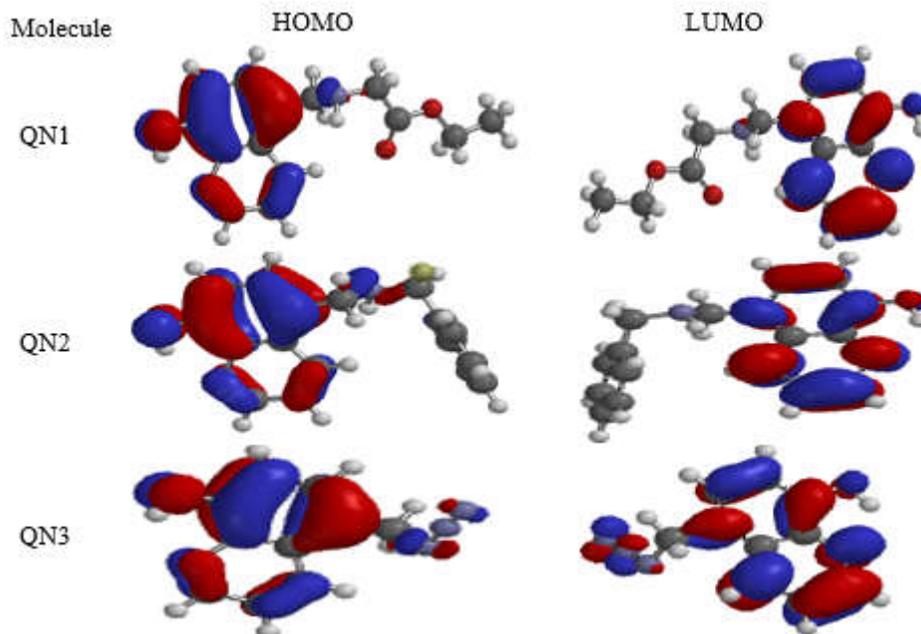
Where  $Y_{\text{obs}}$  = experimentally observed %IE,  $Y_{\text{cal}}$  = calculated %IE,  $\bar{Y}_{\text{obs}}$  = average of the experimentally observed %IE,  $N$  = no of compounds observed,  $P$  = no of molecular descriptors used in the QSAR model and  $R^2$  = Squared coefficient correlation.

## RESULTS AND DISCUSSION

**Quantum Molecular Descriptors:** Several molecular descriptors namely;  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$ , BG (energy gap or band gap), DM (dipole moment),  $\eta$  (chemical hardness),  $\chi$  (electronegativity),  $\omega$  (electrophilicity index),  $\varepsilon$  (global nucleophilicity),  $\Delta N$  (number of electron transfer), energy of back donation ( $\Delta E_{\text{b-d}}$ ), initial molecule-metal interaction energy ( $\Delta\psi$ ), MW (Molecular weight), and V (Volume), were calculated and the results obtained are shown in Table 1. Experimental inhibition efficiency (%IE) obtained from literature (Lgaz *et al.*, 2016) is also shown in Table 1. The effect of the molecular descriptors on the order of the inhibition efficiencies will be discussed here.  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  are quantum chemical parameters that indicate the ability of a molecule to donate electron and the ability of a molecule to accept electron respectively. It has been shown that molecules with high value of  $E_{\text{HOMO}}$  would donate electrons to the metal surface with empty molecular orbital, facilitate the adsorption process and therefore lead to good inhibition performance. Similarly a low value of  $E_{\text{LUMO}}$  will be required for higher inhibition efficiency (Obot *et al.*, 2015). QN3 with the highest  $E_{\text{HOMO}}$  value and the lowest  $E_{\text{LUMO}}$  value has the highest inhibition efficiency, on the other hand QN1 with the lowest  $E_{\text{HOMO}}$  value and the highest  $E_{\text{LUMO}}$  value has the least inhibition efficiency. The order of increasing inhibition efficiency based on the calculated values of  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  (Table 1) is QN3 > QN2 > QN1, which is consistent with the order obtained from experimental values. HOMO and LUMO overlay for the orbitals of the studied molecules are displayed in Figure 2.

**Table 1:** Molecular Descriptors Obtained for the Quinoline Derivatives

	$E_{\text{HOMO}}$ (eV)	$E_{\text{LUMO}}$ (eV)	BG (eV)	DM (Debye)	$\eta$	$\sigma$	$\chi$	$\omega$	$\varepsilon$	$\Delta N$	$\Delta E_{\text{el}}$ (eV)	$\Delta \psi$	MW (amu)	V ( $\text{\AA}^3$ )	%IE
QN1	-5.83	-1.43	4.4	6.03	2.20	0.46	3.63	2.99	0.34	0.77	-0.55	1.29	260.29	267.77	86
QN2	-5.75	-1.49	4.26	4.48	2.13	0.47	3.62	3.08	0.33	0.79	-0.53	1.34	264.33	284.40	88
QN3	-5.72	-1.80	3.92	2.79	1.96	0.51	3.76	3.61	0.28	0.83	-0.49	1.34	200.20	192.06	90

**Fig 2:** The HOMO and LUMO orbitals overlay for QN1, QN2 and QN3

Energy gap (BG) is a key molecular descriptor which gives information about the reactivity of the inhibitor molecule adsorbed on the metallic surface. When ionization energy required to remove an electron from the last occupied orbital is low the value of energy gap will be low. A lower value of energy gap signifies higher reactivity of the inhibitor, which will translate to a higher binding ability of the inhibitor on the surface of the metal (Ebenso *et al.*, 2010). From the result, QN3 has the lowest energy gap and could act as a better corrosion inhibitor. Molecular reactivity can further be measured by chemical hardness and softness of a molecule. Chemical hardness can be defined as the resistance against electron cloud polarization of a chemical species. A hard molecule has a large energy gap and a soft molecule has a small energy gap. Hence very efficient inhibitors are expected to have lower value of chemical hardness and greater value of softness (Erdogan *et al.*, 2017). In Table 1 the order of reactivity based on energy gap, chemical hardness and softness is QN3>QN2>QN1. This is in agreement with the experimental inhibition efficiency order. The correlation between dipole moment and corrosion inhibition efficiency of a compound is not well defined. Some authors reported that increase in dipole moment enhance corrosion inhibition efficiency of a compound (Benali *et al.*, 2007; Sahin *et al.*, 2008),

while some others reported that a low value of dipole moment will enhance the binding of inhibitor molecules on the metal surface and hence lead to a higher inhibition efficiency (Bahrami *et al.*, 2010). In this study the inhibition efficiency increases with the decreasing dipole moment of the inhibitors. Electrophilicity index ( $\omega$ ) means the tendency of a molecule to receive electrons, while nucleophilicity ( $\varepsilon$ ) signifies the tendency to donate electrons to others. A molecule with a large electrophilicity value will not be an efficient corrosion inhibitor while a molecule that has a large nucleophilicity value is expected to be an excellent corrosion inhibitor (Guo *et al.*, 2018). As shown in Table 1, there is an inverse relationship between the Electrophilicity index and the experimental inhibition efficiency.

$\Delta N$  describes the propensity of a molecule to donate electrons and the greater the value of  $\Delta N$ , the greater the propensity of a molecule to donate electrons to the electron poor species. According to Lukovits *et al.*,(2001) if  $\Delta N < 3.6$ , the inhibition efficiency increased with increasing electron donating ability at the metal surface. It was also pointed out that the positive number of electrons transferred ( $\Delta N$ ) indicates that the molecules act as an electron acceptor, while a negative number of electrons

transferred ( $\Delta N$ ) indicates that the molecules act as electron donors. From Table 1, values of  $\Delta N$  for the studied molecules are  $< 3.6$  eV and are all positive, suggesting that all the studied molecules are good electron acceptors, resulting in good inhibition efficiency. The order of increasing inhibition efficiency will be  $QN3 > QN2 > QN1$ , and this is in good agreement with the experimental studies. Gomez *et al.*, (2006), proposed a simple charge transfer theory for donation and back-donation of charges. As stated in equation 7, when the electron transfer and back-donation processes occur at the same time, the energy change is directly proportional to the hardness of the inhibitor molecule. This means that when  $\eta > 0$ , and  $\Delta E_{b-d} < 0$ , back-donation from the molecule to the metal is energetically favored. Based on this, it is evident that  $\Delta E_{b-d}$  will increase while hardness decreases. As shown in Table 1, the calculated  $\Delta E_{b-d}$  increases as the %IE increases.

The initial molecule-metal interaction  $\Delta\psi$  is another significant parameter introduced by Kovacevic and Kokalj (2011). In this study the calculated value of  $\Delta\psi$  revealed that the higher the value of  $\Delta\psi$  the higher the ability of the molecule to be absorbed on the metal surface and hence the higher the inhibition efficiency of the molecule. The order of increasing value of  $\Delta\psi$  is  $QN3 = QN2 > QN1$ , which does not completely agree with the observed trend of %IE. This may suggest that  $\Delta\psi$  is not a sensitive parameter as others discussed above.

**QSAR Analysis:** One molecular descriptor (dipole moment) was selected for the QSAR model and this was done in order to avoid multi-collinearity. The %IE predicted through QSAR model replicated the experimental %IE well as shown in Table 3 and Figure 3, with fitting factor ( $R^2$ ) 0.9993. The analysis was further validated by using  $CV.R^2$  and  $R^2_{adj}$ . As shown in Table 3, the calculated  $CV.R^2$  (0.9994) indicated the reliability, acceptability and appropriateness of the developed QSAR model, since the value is greater than 0.5 which is the standard (Marrero, 2004). Moreso, the  $R^2_{adj}$  (0.9988) explained that the QSAR model developed is predictive because it is greater than 0.6 (Standard).

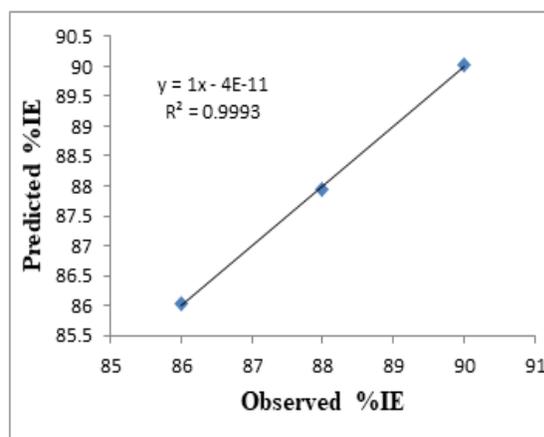
$$\%IE = 93.4698 - 1.23380(DM)$$

**Table 2:** Observed and Calculated % Inhibition Efficiency

Inhibitors	Observed %IE	Predicted %IE	Residual
QN1	86	86.03	-0.03
QN2	88	87.94	0.06
QN3	90	90.03	-0.03

**Table 3:** Statistical Parameters for Validation of QSAR Model

N	P	$R^2$	$CV.R^2$	$R^2_{adj}$
3	1	0.9993	0.9994	0.9988



**Fig 3:** Correlation between experimental and predicted %IE

**Conclusion:** The results showed that studied quinoline derivatives will be effective in terms of the prevention of corrosion of mild steel in acidic solution. The QSAR model developed reproduced the observed inhibition efficiency of these compounds well. The results obtained and the discussions made in this study are important for the synthesis and rational design of new quinoline derivatives for corrosion inhibition in future studies.

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