CORROSION INHIBITION STUDY ON (Z)-N'-(1-PHENYLETHYLIDENE) BENZOHYDRAZIDE DERIVATIVES ON CARBON STEEL IN ACIDIC SOLUTIONS

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ABSTRACT

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Decomposition of carbon steel via corrosion process has caused a serious damage to several organisations worldwide. Despite efforts put in place to curb this menace by scientists, havoc caused by corrosion of metal still remain. Therefore, in a way to find effective corrosion inhibitor, (Z)-N'-(1-phenylethylidene) benzohydrazide derivatives was optimised using density functional theory and the obtained molecular descriptors correlated well with the experimental percentage inhibition efficiency. Also, the developed quantitative structure-activity relationship study (QSAR) model revealed that dipole moment impeccably define anti-corrosion properties of (Z)-N'-(1-phenylethylidene) benzohydrazide Derivatives.

Keywords: (Z)-N'-(1-phenylethylidene) benzohydrazide, carbon steel, corrosion, QSAR.

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INTRODUCTION

The part played by carbon steel in most industrial processes cannot be over emphasized (Abd El-Lateef et al., 2016; Erazua et al., 2019). As reported by many researchers, the rate at which many industries such as mechanical companies, construction companies etc., place demand on carbon steel is great and this could be due to its low cost and extraordinary mechanical strength (Negma et al., 2012; Ulaeto et al., 2012; Oyebamiji et al., 2018). But, rusting of carbon steel led to prickling of its surface (Oyebamiji & Adeleke, 2018); thus, this made it to become useless for industrial purpose which in turn adds to economic fatalities (Kavitha & Gunavathy, 2014).

Benzohydrazide derivatives have been reported to be useful by several scientists as analgesic, anti-microbial, anti-cancer agents (Zhong et al., 2007; Liu et al., 2011; Bhole & Bhusari, 2011; Bhole et al., 2012). Also, hydrazide derivatives are vital compounds in producing hydrazones as well as some heterocyclic compounds (Alhadi et al., 2015; Jiang & Yan, 2016).

According to Prakash (2018), hydrazide derivatives also act as prospective corrosion inhibitors against several metals (Prakash, 2018).

Thus, this research is aimed at identifying the descriptors which describe anti-corrosion activity of (Z)-N'-(1-phenylethylidene) benzohydrazide Derivatives (Fouda et al., 2014) using density functional theory as well as quantitative structural activities relationships method. The studied compounds are (Z)-2-chloro-N'-(1-(2-hydroxyphenyl)ethylidene) benzohydrazide (**A**), (Z)-N'-(1-(2-hydroxyphenyl)ethylidene)-2-methylbenzohydrazide (**B**), (Z)-N'-(1-(2-hydroxyphenyl)ethylidene)-2-methoxybenzohydrazide (**C**).

METHODOLOGY

The studied derivatives of (Z)-N'-(1-phenylethylidene) benzohydrazide (Figure 1) were optimized using density functional theory method via Spartan 14 (Geerlings et al., 2003). The obtained descriptors E_{LUMO} (lowest unoccupied molecular orbital energy revealed the ability of compounds to receive electron from neighbouring compounds), E_{HOMO} (highest occupied molecular orbital energy revealed the capability of compounds to donate electron from neighbouring compounds), global electrophilicity (ω), chemical potential (μ) (disclose the rate of change of free energy of a thermodynamic system with respect to the change in the number of molecules of the species that are added to the system), chemical hardness (η), electronegativity (χ), electron affinity, local reactivity index, and ionization potential) which describe anti-corrosion activities of the studied compounds were calculated and reported. The chemical indices which is a function of E_{HOMO} and E_{LUMO} that were related to Koopmans' theorem (Geerlings et al., 2003) were defined by the equation 1, 2, 3:

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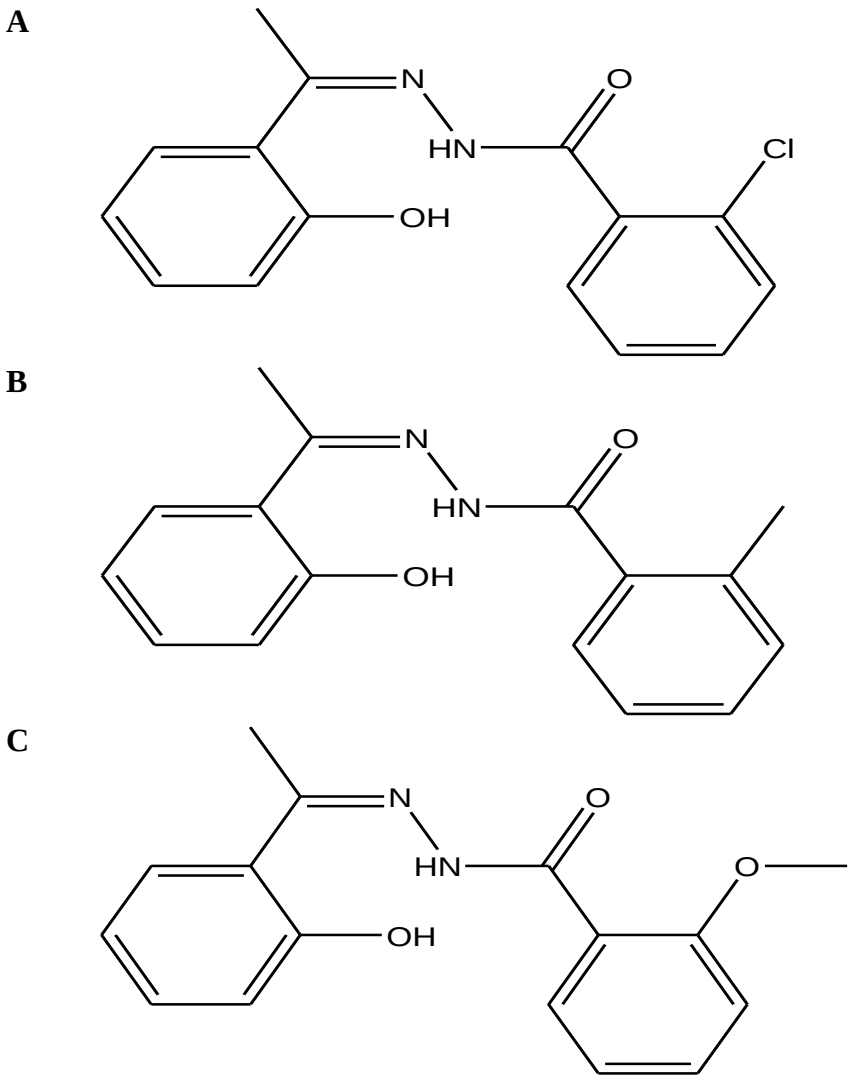

Figure 1. Structures of (Z)-N'-(1-phenylethylidene) benzohydrazide Derivatives (Fouda et al., 2014).

Chemical hardness (ŋ): $\frac{1}{2}(E_{LUMO} - E_{HOMO}) - - - - - - - - - - - - - - - (1)$

Chemical potential and electronegativity are defined as: $\chi = -\mu = -\frac{1}{2}(E_{LUMO} + E_{HOMO}) - (2)$

Global electrophilicity: $\omega = \frac{\mu^2}{2\eta} - (3)$

The calculated electrons transfer (ΔN) was calculated as; $\Delta N = \frac{\chi_{Fe} - \chi_{inh}}{2(\eta_{Fe} + \eta_{inh})} - - - - - (4)$

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χ_{Fe} and χ_{inh} denotes electronegativity of metal (7 $eVmol^{-1}$) and the studied inhibitor (0 $eVmol^{-1}$) respectively (Musa et al., 2010; Oyebamiji & Semire, 2018). The local reactivity index of compounds with anti-corrosion properties explains the reactivity of a certain atom and Fukui function helps its estimation. Therefore, equation 5 reveals the mathematical expression for Fukui functions can be mathematically expressed using equation 5 and 6 (Zhou & Navangul, 1990);

$$f_{(r)}^{+} = P_{N+1(r)} P_{N(r)} \text{----------(5)}$$

$$f_{(r)}^{-} = P_{N(r)} - P_{N-1(r)} \text{----------(6)}$$

$f_{(r)}^{+}$ and $f_{(r)}^{-}$ reveal the point at which nucleophilic and electrophilic attack occur respectively. Also, $P_{N(r)}$, $P_{N-1(r)}$ and $P_{N+1(r)}$, indicate the electronic densities of neutral, cationic and anionic species respectively.

Quantitative Structure Activity Relationship (QSAR) analyses

The role played by effective molecular descriptors in developing predictive quantitative structure-activity relationship (QSAR) model cannot be overemphasized (Olofinjana et al., 2017). The obtained descriptors from optimised studied compounds were screened and used in developing QSAR model using multiple linear regression method. The observed percentage inhibition efficiency (%IE) was used as dependent variable while the calculated descriptors were used as independent variables. The studied QSAR analysis was carefully executed so as to avoid multi-collinearity. Also, series of statistical factors (cross validation (R_2) and adjusted R_2) were calculated for QSAR model validation (Equation 7 and 8).

$$\boldsymbol{C_v.R^2 = 1 - \frac{\Sigma(Y\,obs - Y\,cal)^2}{\Sigma(Y\,obs - \bar{Y}obs)^2}} \text{----------(7)}$$

Note: Y_{obs} =observed percentage inhibition efficiency (%IE), Y_{cal}= predicted percentage inhibition efficiency.

$$\boldsymbol{R_a^2 = \frac{(N-1)\times R^2 - P}{N-1-P}} \text{----------(8)}$$

Note: N = total number of studied compounds, R^2= Sample correlation coefficient, p=*number of predictors.*

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RESULTS AND DISCUSSION

Calculated Molecular Descriptors

According to Wang et al., (2004), adsorption ability of a compound is a function of its calculated molecular descriptors and inhibition efficiency (Wang et al., 2004). In this work, several descriptors which describe anti-corrosion inhibition activity obtained from the studied compounds were displayed in Table 1. The descriptors obtained were E_{HOMO} (eV), the E_{LUMO} (eV), band gap (eV), dipole moment (Debye), the chemical hardness (η), chemical potential, global nucleophilicity, area ($Å^2$), volume ($Å^3$), molecular weight (amu), Ovality (Table 1).

Table 1. Molecular descriptors obtained from (Z)-N'-(1-phenylethylidene) benzohydrazide Derivatives using 6-31G basis set.**

Parameters	A	B	C
E_{HOMO}(eV)	-5.76	-5.75	-5.58
E_{LUMO} (eV)	-1.37	-1.15	-1.21
Energy gap(ΔE)	4.39	4.60	4.37
Chemical hardness(η)	2.19	2.30	2.18
Chemical potential	-3.56	-3.45	-3.39
Electrophilicity index(ω)	2.88	2.58	2.62
Electron transferred(ΔN)	0.78	0.77	0.83
Dipole moment(Debye)	4.16	5.36	5.52
Area	301.93	306.05	316.15
Volume	280.47	284.90	293.77
Ovality	1.46	1.46	1.48
PSA	48.16	48.62	52.11
POL	63.09	63.40	64.17
Percentage Inhibition Efficiency (%IE)	76.99	83.1	84.88

E_{HOMO} reveals the ability of organic inhibitor to release electron to the nearby compounds (Musa et al., 2010). High E_{HOMO} value of compound showed it tendency to inhibit carbon steel and it also proof of its ability to adsorb well. Therefore, higher E_{HOMO} value has helped compound **C** to inhibit than other studied compounds. Also, the calculated E_{LUMO} reveal the capability of compounds to admit electron from nearby molecules and as reported by many researchers (Semire & Oyebamiji, 2017), lower E_{LUMO} helps the ability of compound to receive electron from the neighbouring compounds. Therefore, no correlation was observed between compound **C** with highest experimental inhibition efficiency and the calculated E_{LUMO}.

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Moreover, band gap reveals the level of reactivity of molecular compound. Also, lower band gap enhances the reactivity of a compound (Eddy, 2010). Therefore, it is expected that compound C with lower band gap will react better with carbon steel than other studied compounds. E_{HOMO}-E_{LUMO} overlay for (Z)-N'-(1-phenylethylidene) benzohydrazide Derivatives were displayed in Figure 2. Also, dipole moment is an important directory which assists in envisaging route of a corrosion inhibition (Gece, 2008). According to Abdulazeez et al., (2016), better molecular absorptivity of organic inhibitors on carbon steel is also a function of increase in dipole moment (Abdulazeez et al., 2016); thus, as shown in Table 1, it is expected that compound C with increased dipole moment will inhibit than other studied compounds. As shown in Table 1, it was observed that percentage inhibition concentration increases as dipole moment increases.

More so, the calculated electron transfer reveals the ability of organic inhibitor to release electron to the nearby compounds. It was also reported by Gomez et al., (2006), that increasing rate of electron transferred by organic inhibitors is a proof of it tendency to release electron to the neighbouring molecules which have the ability to receive it. It was also observed that the ability of compound C to donate electron agreed with Lukovits's study (Lukovits et al., 2001). Therefore, compound C with highest value of electron transfer shows that it has the tendency to inhibit than other studied compounds. Also, it was shown that electron transfer for compound **C** correlates with the highest percentage inhibition efficiency (%IE) reported in Table 1. Similarly, increasing chemical potential, area, volume, ovality, polar surface area and polarizability seemed to boost inhibition efficiency of compound **C** as shown in Table 1. More so, increasing chemical potential showed the level of stability of the chemical compounds (Gibbs, 1876), therefore, reaction between compound C and carbon steel is more stable than reaction between compound A and B together with carbon steel.

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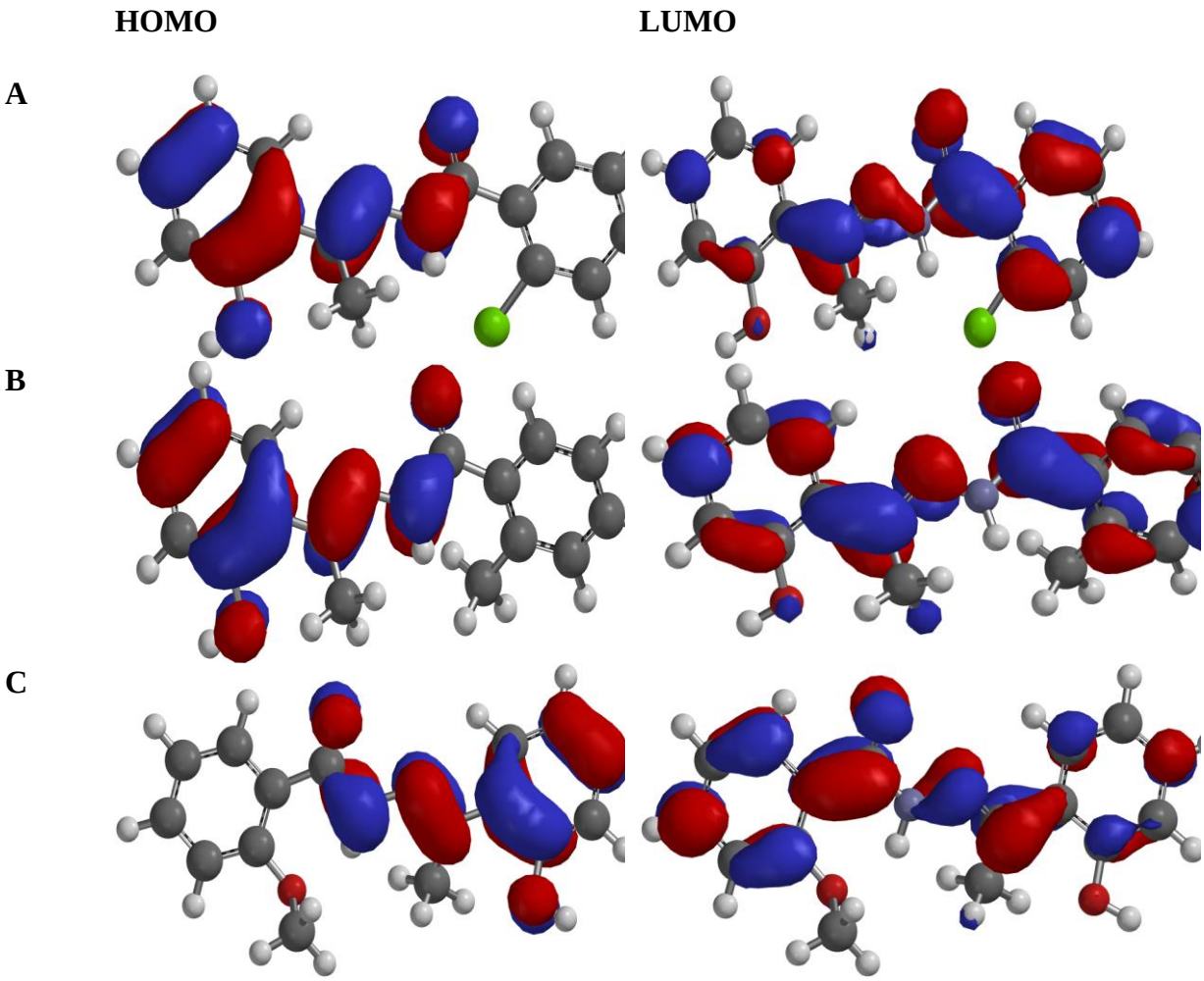

Figure 2. HOMO-LUMO overlay for (Z)-N'-(1-phenylethylidene) benzohydrazide derivatives.

Calculated Fukui Function

Fukui function as a function that explains the frontier orbital could be used to investigate local reactivity of organic inhibitors. It also helps in locating electrophilic (f^-) and nucleophilic (f^+) point of attacks in molecular compounds. As shown in Tables 2-4, the point at which f^- have the highest values shows the area where electrophilic attack could possibly occur whereas the point at which f^+ possess the highest value reveal the location where nucleophilic attack could possibly take place. In this work, for compound **A**, electrophilic and nucleophilic attack occurs at C5 (0.037) and C15 (0.013**)** respectively whereas for compound **B**, electrophilic and nucleophilic attack occurs at C2 (0.006) and C15 (0.014). Also, for compound C, the highest values for electrophilic and nucleophilic were located at C16

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(0.017) and (0.023) respectively. Therefore, it was observed that compound A and B have nucleophilic attack on C15 but electrophilic attack on different location.

Table 2. Fukui function indices for nucleophilic and electrophilic attacks for compound A.

Atom	$P_{N(r)}$	$P_{N+1(r)}$	$P_{N-1(r)}$	f^+	f^-
C(1)	-0.090	-0.106	-0.083	-0.016	-0.007
C(2)	0.048	0.029	0.041	-0.019	0.007
C(3)	-0.146	-0.165	-0.147	-0.019	0.001
C(4)	-0.069	-0.073	-0.062	-0.004	-0.007
C(5)	-0.075	-0.112	-0.063	-0.037	**0.037**
C(6)	-0.088	-0.096	-0.081	-0.008	-0.007
C(7)	0.567	0.505	0.576	-0.062	-0.009
C(8)	0.248	0.201	0.290	-0.047	-0.042
C(9)	0.062	0.066	0.076	0.004	-0.014
C(10)	-0.087	-0.114	-0.057	-0.027	-0.030
C(11)	0.280	0.255	0.323	-0.025	-0.043
C(12)	-0.104	-0.126	-0.088	-0.022	-0.016
C(13)	-0.095	-0.096	-0.073	-0.001	-0.022
C(14)	-0.129	-0.137	-0.114	-0.008	-0.015
C(15)	-0.387	-0.374	-0.401	**0.013**	0.014
N(1)	-0.403	-0.399	-0.339	0.004	-0.064
N(2)	-0.269	-0.303	-0.216	-0.034	-0.053
O(1)	-0.480	-0.553	-0.411	-0.073	-0.069
O(2)	-0.567	-0.573	-0.517	-0.006	-0.050
Cl(1)	-0.019	-0.092	0.011	-0.073	-0.030

Table 3. Fukui function indices for nucleophilic and electrophilic attacks for compound B.

Atom	$P_{N(r)}$	$P_{N+1(r)}$	$P_{N-1(r)}$	f^+	f^-
C(1)	-0.091	-0.103	-0.083	-0.012	-0.008
C(2)	-0.014	-0.023	-0.020	-0.009	**0.006**
C(3)	0.100	0.086	0.108	-0.014	-0.008
C(4)	-0.125	-0.129	-0.120	-0.004	-0.005
C(5)	-0.073	-0.104	-0.060	-0.031	-0.013
C(6)	-0.095	-0.103	-0.088	-0.008	-0.007
C(7)	0.531	0.472	0.537	-0.059	-0.006
C(8)	0.245	0.194	0.286	-0.051	-0.041

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Atom	$P_{N(r)}$	$P_{N+1(r)}$	$P_{N-1(r)}$	f^+	f^-
C(9)	0.063	0.065	0.076	0.002	-0.013
C(10)	-0.087	-0.119	-0.058	-0.032	-0.029
C(11)	0.279	0.250	0.320	-0.029	-0.041
C(12)	-0.105	-0.130	-0.089	-0.025	-0.016
C(13)	-0.095	-0.095	-0.074	0.000	-0.021
C(14)	-0.129	-0.139	-0.115	-0.010	-0.014
C(15)	-0.389	-0.375	-0.403	**0.014**	-0.014
C(16)	-0.394	-0.382	-0.411	0.012	-0.061
N(1)	-0.398	-0.391	-0.333	0.007	-0.065
N(2)	-0.263	-0.310	-0.213	-0.047	-0.050
O(1)	-0.476	-0.548	-0.412	-0.072	-0.064
O(2)	-0.568	-0.576	-0.521	-0.008	-0.047

Table 4. Fukui function indices for nucleophilic and electrophilic attacks for compound C.

Atom	$P_{N(r)}$	$P_{N+1(r)}$	$P_{N-1(r)}$	f^+	f^-
C(1)	-0.018	-0.143	-0.110	-0.025	-0.008
C(2)	0.015	0.005	0.008	-0.010	0.007
C(3)	0.278	0.242	0.292	-0.036	-0.014
C(4)	-0.096	-0.104	-0.090	-0.008	-0.006
C(5)	-0.089	-0.127	-0.077	-0.038	-0.012
C(6)	-0.086	-0.088	-0.078	-0.002	-0.008
C(7)	0.597	0.529	0.610	-0.068	-0.013
C(8)	0.244	0.195	0.289	-0.049	-0.045
C(9)	0.063	0.067	0.073	0.004	-0.01
C(10)	-0.088	-0.115	-0.058	0.010	-0.03
C(11)	0.277	0.251	0.319	-0.026	-0.042
C(12)	-0.105	-0.127	-0.089	-0.022	-0.016
C(13)	-0.095	-0.096	-0.077	-0.001	-0.018
C(14)	-0.129	-0.398	-0.116	-0.269	-0.013
C(15)	-0.381	-0.368	-0.396	0.013	0.015
C(16)	-0.085	-0.062	-0.102	**0.023**	**0.017**
N(1)	-0.452	-0.447	-0.380	0.005	-0.072
N(2)	-0.265	-0.301	-0.214	-0.036	-0.051
O(1)	-0.495	-0.566	-0.430	-0.071	-0.065
O(2)	-0.569	-0.575	-0.524	-0.006	-0.045
O(3)	-0.562	-0.563	-0.571	-0.001	0.009

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Quantitative Structure Activity Relationship (QSAR) Study

This study described the relationship between calculated molecular descriptors and percentage inhibition efficiency of organic inhibitors. Multiple linear regression via ordinary least square method was employed to develop effective QSAR model. The QSAR model developed comprises of only dipole moment; this was done to avoid multicollinearity and to achieve better predicting ability (Equation 9). In this work, it was observed that the developed model has the ability to predict well as revealed by the obtained squared correlation coefficient (R^2). Since it has been observed from many research that squared correlation coefficient (R^2) alone cannot be used to judge the validity of the developed QAR model, therefore, calculated adjusted squared correlation coefficient, P-value and mean square error and mean square error (MSE) were used to validate the developed model. This was also confirmed via the predicted percentage inhibition efficiency as shown in Table 5 as the predicted %IE were closer to the experimental %IE. More so, it was observed from equation 9 that increasing dipole moment leads to increase in percentage inhibition efficiency (%IE).

Table 5. Experimental and predicted % inhibition efficiency.

	Experimental %IE	**Predicted %IE**	**Residual**
A	76.99	76.93	0.06
B	83.10	83.58	-0.48
C	84.88	84.46	0.42

More so, four compounds with (Z)-N'-(1-phenylethylidene) benzohydrazide as the parent compound (Table 6) were proposed and their inhibitory efficiencies were predicted using the developed model (Equation 9). This was also executed to confirm the validity and reliability of the developed model. According to the reported %IE shown in Table 6, it was observed that the proposed compounds have better ability to inhibit than the model compounds used in this work. In this work, addition of NO_2, Br, F and I to the parent compound proved to greatly enhance the percentage inhibition efficiency of (Z)-N'-(1-phenylethylidene) benzohydrazide. As shown in Table 6, the predicted percentage inhibition efficiency for the proposed compounds 1 – 4 were 98.40, 88.66, 87.78 and 88.44 and it was confirmed that addition of NO_2 to the parent compound greatly enhanced the ability of (Z)-N'-(1-phenylethylidene) benzohydrazide to inhibit rusting.

%IE = 53.9115 + 5.53427(Dipole moment) ----------(9)

R^2=0.988, Adjusted R^2= 0.976, P < 0.0001, MSE= 0.13492,

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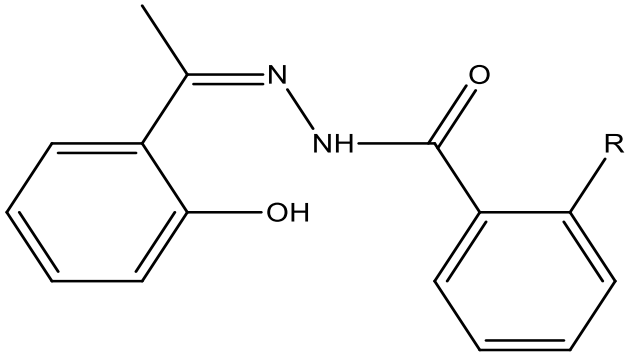

Figure 3: Parent compound for proposed inhibitors

Table 6. Predicted % inhibition efficiency for proposed compounds.

	R	Predicted %IE
1	NO_2	98.40
2	Br	88.66
3	F	87.78
4	I	88.44

CONCLUSION

The role played by benzohydrazide derivatives in scientific world cannot be overemphasized. Also, series of molecular descriptors obtained from optimization of (Z)-N'-(1-phenylethylidene) benzohydrazide derivatives correlated well with experimental percentage inhibition efficiency. It was observed that the screened descriptors (increasing E_{HOMO}, Chemical Potential and Electron transferred (ΔN)) describe anti-corrosion activities of the studied compound well. Also, the develop QSAR model proved to be effective via the calculated predicted percentage inhibition efficiency and this proved the efficiency of the developed model in predicting the percentage inhibition efficiency of another set of proposed compounds.

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