Quantum chemical studies on inhibition activities of 2,3-dihydroxypropyl-sulfanyl derivative on carbon steel in acidic media

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Abstract

The inhibiting activity of 3 sets of organic compounds ([2-[(2,3-dihydroxypropyl)sulfanyl]-N-octylacetamide (**DSO**), 2-[(2,3-dihydroxypropyl)sulfanyl]-N-decylacetamide (**DSD**) and 2-[(2,3-dihydroxypropyl)sulfanyl]-*N*-dodecylacetamide (**DSDD**)) were studied. The studied anti-corrosion compounds i.e. 2,3-dihydroxypropyl-sulfanyl derivatives were calculated using quantum chemical calculation and several descriptors (highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}) and chemical reactivity indices (global electrophilicity index (ω), chemical hardness (η), electronegativity (χ), local reactivity index, electron affinity and ionization potential) which described the anti-corrosion properties of the studied compounds were obtained. Fukui Indices for nucleophilic and electrophilic Attacks for inhibitors i.e. [2-[(2,3dihydroxypropyl)sulfanyl]-N-octylacetamide (DSO), 2-[(2,3-dihydroxypropyl)sulfanyl]-Ndecylacetamide and 2-[(2,3-dihydroxypropyl)sulfanyl]-N-dodecylacetamide (DSD) (DSDD) were observed and sites for nucleophilic and electrophilic attacks for DSO were C6 (0.047) and O3 (0.170); for **DSD**, the utmost value for f_k^+ was found on C6 (0.047), and the highest value for f_k^- was located on C5 with 0.099 while the greatest value for f_k^+ was situated on C6 with 0.047 and the highest value for f_k^- is found on C3 and C4 with 0.053 each for the **DSDD** molecule. The molecules used in this study was calculated using quantum chemical calculation and it was achieved using Spartan 14. More so, the QSAR study using multiple linear regression method was executed using Gretl 1.9.8. The selected descriptors among the entire calculated descriptors were used in the development of quantitative structural activity relationship (QSAR) model and the developed model replicated the observed %IE. The correlation coefficient (R^2) was calculated to be 0.926, cross validation (CV.R²) was 0.963 and adjusted R^2 was 0.852. Also, E_{LUMO} was the predominating parameter in the corrosion inhibition property of the studied compounds.

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1. Introduction

The use of molecular organic compounds that contain heteroatom like nitrogen as well as oxygen as a corrosion inhibitors against carbon steel in acidic media has receive a number of attention in academic world and industries [1]. The means of inhibiting corrosion by these organic compounds is via adsorption on the surface of metals [2-4]. Thus, the efficiency of the organic compounds used as corrosion inhibitors is a function of the rate at which they are adsorbed as well as their ability to shield metal surfaces [5]. Mouhsine *et al.*, 2017 and Noor *et al.*, 2008 reported that several factors influence the adsorption of corrosion inhibitors on the surface of metals. Such factors include the nature and concentration of organic compounds used as inhibitor as well as the temperature [6, 7].

The global use of carbon steel in industries such as the construction of pipelines for transferring fluids has gained the attention of researchers world-wide [8, 9]. Carbon steel get corroded naturally in moist and acidic places which are stimulated by acid wash, which then resulted into prickling of metal surface; *i.e.*, the environmental effect on metals cause corrosion [10].

The use of quantum chemical methods has greatly demonstrated a high level of efficiency in the determination of molecular structure of organic compounds and their property electronic properties as well as the level of reactivities of such compounds [11]. Also, quantum chemical calculation via density functional theory (DFT) has been proficiently used by several researchers to obtain deeper insight into chemical reactivity and selection of the point of attraction of the molecular compounds. In addition, the use of quantum chemical method in corrosion study provides insight into the nature and structure of anti-corrosion properties of studied compounds [12, 13].

In this work, molecular descriptors of three molecular compounds [2-[(2,3-dihydroxypropyl)sulfanyl]-N-octylacetamide (**DSO**), 2-[(2,3-dihydroxypropyl)sulfanyl]-N-decylacetamide (**DSD**) and 2-[(2,3-dihydroxypropyl)sulfanyl]-N-dodecylacetamide (**DSDD**) (Figure 1)] which have been experimentally studied by Serkan*et al.*, 2018, were examined using quantum chemical method via density functional theory so as to probe theoretically into their anticorrosion properties on carbon steel [14].



n =6 for DSO; n= 8 for DSD; n=10 for DSDD

Figure 1. Schematic structures of the studied compounds [14].

2. Methodology

Quantum chemical calculations were executed using Spartan 14 software via 6-31G* as basis set [15] because of its dependability in calculating efficient molecular descriptors. Theoretical descriptors like highest occupied molecular orbital energy ($E_{\rm HOMO}$), lowest unoccupied molecular orbital energy ($E_{\rm LUMO}$) and chemical reactivity indices (global electrophilicity index (ω), chemical hardness (η), electronegativity (χ), local reactivity index, electron affinity and ionization potential) were calculated. The chemical indices were defined based on $E_{\rm HOMO}$ and $E_{\rm LUMO}$ that were linked to Koopmans' theorem [16] by using Equations 1, 2 and 3:

Chemical potential and electronegativity are related as:

$$\chi = -\mu = \left(\frac{\delta E}{\delta N}\right)_{\nu(r)} = \frac{1}{2}(IE + EA) = -\frac{1}{2}(E_{\text{LUMO}} + E_{\text{HOMO}})$$
(1)

Chemical hardness (η): this is a property to examine the stability and reactivity of molecular compounds. This is mathematically expressed in Equation 2.

$$\eta = \left(\frac{\delta^{2}E}{\delta N^{2}}\right)_{\nu(r)} = \frac{1}{2}(IE - EA) = \frac{1}{2}(E_{\text{LUMO}} - E_{\text{HOMO}})$$
(2)

Global electrophilicity ($\boldsymbol{\omega}$): this reveals the electrophilic proclivity of compounds (Equation 3).

$$\omega = \frac{\mu^2}{2\eta} \tag{3}$$

Number of electrons transfer (ΔN) was mathematically expressed in Equation 4.

$$\Delta N = \frac{\chi_{Fe} - \chi_{inh}}{2(\eta_{Fe} + \eta_{inh})} \tag{4}$$

The electronegativity of metal and corrosion inhibitors were denoted by χ_{Fe} (7.0 eV mol⁻¹) and χ_{inh} respectively [17, 18]. More so, η_{Fe} (0 eV mol⁻¹) and η_{inh} designate the hardness of metal (Fe) and the molecular compounds (inhibitor) [19]. The local reactivity index of corrosion inhibitors clarifies the reactivity of a definite atom and this could be evaluated using Fukui function. However, the disparity in electron density for $f_{(r)}^+$ and $f_{(r)}^-$ (nucleophile) as the Fukui functions can be mathematically expressed using equation 5 and 6 [20];

$$f_{(r)}^{+} = P_{N+1(r)} - P_{N(r)}$$
 (for a nucleopilic attack) (5)

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

 $P_{N+1(r)}$, $P_{N-1(r)}$ and $P_{N(r)}$ signify the electronic densities of anionic, cationic and neutral species respectively.

2.1 Descriptor selection and QSAR Model Analysis

In quantitative structure activity relationship (QSAR) study, parameters with high predicting power is required for development of QSAR model [21, 22]. The QSAR model was developed via multiple linear regression method. The predicted inhibitory activity was calculated using partial least square method. The software used for partial least square method was XLSTAT 2018.

2.2 Validation of QSAR Model

Cross validation $(C_{\nu}.R^2)$ and adjusted $R^2(R_{adj}^2)$ as shown in Equation 7 and 8 were used for the assessment of the validation of developed QSAR model.

$$C_{\nu} R^{2} = 1 - \frac{\sum (Y_{\rm obs} - Y_{\rm cal})^{2}}{\sum (Y_{\rm obs} - \bar{Y}_{\rm obs})^{2}}$$
(7)

The adjusted R^2 could be calculated using equation (8)

$$R_{\rm a}^2 = \frac{(N-I) \times R^2 - P}{N-1-P}$$
(8)

The developed QSAR model is considered predictive, if C_v . $R^2 > 0.5$ and $R_{adj}^2 > 0.6$ [23, 24].

3.0 Results and Discussion

3.1. Molecular descriptors

Table 1 contains the values of the molecular descriptors obtained by using quantum chemical method via density functional theory. The molecular parameters included E_{HOMO} (eV), the E_{LUMO} (eV), band gap (eV), dipole moment (Debye), the chemical hardness (η), chemical potential, global nucleophilicity, area (Å²), volume (Å³), log *P*, molecular weight (amu), Ovality, electron transfer and polarizability.

 Table 1. Selected molecular descriptors obtained by B3LYP/6-31G*.

	номо	LUMO	BG	DM	СН	СР	MW	LOG P	AREA	VOL	OVA	POL	%IE
DSO	-6.22	0.25	6.47	7.02	3.235	-2.985	277.43	1.52	345.81	302.51	1.59	64.39	93.74
DSD	-6.21	0.26	6.47	6.96	3.235	-2.975	305.48	2.35	380.43	338.02	1.62	67.27	93.24
DSDD	-6.21	0.26	6.47	6.93	3.235	-2.975	333.54	3.19	423.97	375.70	1.68	70.32	93.38

IE: Experimental inhibition Efficiency, MW: Molecular Weight, VOL: Volume, OVA: Ovality, POL: Polarizability.

The optimized structure for 2,3-dihydroxypropyl-sulfanyl derivative is shown in Figure 2.



Figure 2. Optimized structure of 2,3-dihydroxypropyl-sulfanyl derivative.

The rate at which molecular compounds react with neighbouring molecules could be determined by frontier molecular orbitals (E_{HOMO} and E_{LUMO}) [25]. Also, Fukui (1975) showed that according to frontier molecular orbital theory, the development of a transition state is a function of the relationship between E_{HOMO} and E_{LUMO} of reacting species [26]. High E_{HOMO} reveal the ability of corrosion inhibitors to donate electrons to apposite surrounding compounds that have low energy [27] and it also enhance adsorption [28, 29]. However, no fair correlation exist between the calculated E_{HOMO} and the experimental inhibition efficiencies (Table 1). E_{LUMO} shows the accepting capacity of molecular compound to receive electrons. According to Semire *et al.*, the lower the E_{LUMO} value, the more possible for neighbouring compounds to accept electrons from the metal surface.

Hence, the lowest E_{LUMO} value for **DSO** enhanced its inhibition efficiency over other molecules in this study, *i.e.* there is correlation between E_{LUMO} and the experimental corrosion inhibition efficiency.

Furthermore, energy band gap showed details about the overall reactivity of molecules. Eddy, 2010, reported that lower energy band gap brings about better reactivity of molecules [31]. However, the calculated band gap for **DSO**, **DSD** and **DSDD** are the same as shown in Table 1.

HOMO and LUMO overlay for **DSO**, **DSD** and **DSDD** are displayed in Figure 3.



Figure 3. The HOMO and LUMO orbitals overlay for 2,3-dihydroxypropyl-sulfanyl derivatives.

Dipole moment is also a vital directory that helps in predicting path of a corrosion inhibition [32]. Increase in dipole moment brings about increase in deformability energy and improves the molecule adsorption on metal surface. Therefore, increase in dipole moment leads to increase in corrosion inhibition efficiency [33–36]. As shown in Table 1, there is a fair correlation between the calculated dipole moment and corrosion inhibition efficiency.

Comparison of the calculated dipole moment with observed inhibition efficiency showed that the %IE of 2-[(2,3-dihydroxypropyl)sulfanyl]-N-octylacetamide derivatives increase with increasing dipole moment. Also, decreased chemical Potential, Log P, Area, volume, Ovality and polarizability appeared to enhance the inhibition efficiency of **DSO**.

3.2 Local Reactivity Descriptors

Fukui function could be used to analyse local reactivity of molecular compounds. They also define the sites where electrophilic (f_k^-) , nucleophilic (f_k^+) and radical reactions have the highest prospect to occur in a molecule. According to Sourav *et al.*, 2015, utmost limit values of f_k^+ and f_k^- regulate the nucleophilic and electrophilic attack respectively [37]. Variations in electron density of a compound can be calculated by f_k^+ when molecular compounds receive electron while f_k^- could be used to calculate variation in electron density of compound donate electron.

Fukui functions of 2,3-Dihydroxypropyl-Sulfanyl Derivatives were calculated using Equations 5 and 6 and the results are shown displayed in Tables 2–4.

АТОМ	$P_{N-1(r)}$	$P_{N+1(r)}$	$P_{N(r)}$	f_k^+	f_k^-
C1	0.093	0.119	0.124	-0.005	0.031
C2	-0.073	-0.023	-0.049	0.026	0.024
C3	-0.488	-0.413	-0.434	0.021	0.054
C4	-0.500	-0.436	-0.446	0.010	0.054
C5	0.326	0.213	0.426	-0.213	0.100
C6	-0.117	-0.049	-0.096	0.047	0.021
C7	-0.261	-0.251	-0.263	0.012	-0.002
C8	-0.266	-0.235	-0.252	0.017	0.014
C9	-0.257	-0.242	-0.253	0.011	0.004
C10	-0.265	-0.250	-0.259	0.009	0.006
C11	-0.251	-0.248	-0.248	0.000	0.003
C12	-0.249	-0.251	-0.250	-0.001	-0.001
C13	-0.449	-0.445	-0.447	0.002	0.002
N1	-0.560	-0.664	-0.595	-0.069	-0.035
O1	-0.426	-0.677	-0.677	0.000	-0.251
O2	-0.632	-0.671	-0.666	-0.005	-0.034
O3	-0.673	-0.705	-0.503	-0.202	0.170
S 1	0.650	-0.030	0.068	-0.098	-0.582

Table 2. Fukui indices for nucleophilic and electrophilic attacks for inhibitor DSO.

ATOM	$P_{N-1(r)}$	$P_{N+1(r)}$	$\boldsymbol{P}_{\boldsymbol{N}(\boldsymbol{r})}$	f_k^+	f_k^-
C1	0.093	0.119	0.124	-0.005	0.031
C2	-0.073	-0.023	-0.048	0.025	0.025
C3	-0.489	-0.413	-0.434	0.021	0.055
C4	-0.500	-0.435	-0.446	0.011	0.054
C5	0.326	0.212	0.425	-0.213	0.099
C6	-0.117	-0.049	-0.096	0.047	0.021
C7	-0.261	-0.251	-0.263	0.012	-0.002
C8	-0.266	-0.235	-0.252	0.017	0.014
C9	-0.256	-0.241	-0.252	0.011	0.004
C10	-0.265	-0.250	-0.259	0.009	0.006
C11	-0.256	-0.255	-0.254	-0.001	0.002
C12	-0.257	-0.262	-0.259	-0.003	-0.002
C13	-0.248	-0.249	-0.248	-0.001	0.000
C14	-0.263	-0.255	-0.260	0.005	0.003
C15	-0.446	-0.443	-0.445	0.002	0.001
N1	-0.560	-0.663	-0.595	-0.068	-0.035
O1	-0.673	-0.677	-0.677	0.000	-0.004
O2	-0.631	-0.671	-0.666	-0.005	-0.035
O3	-0.426	-0.704	-0.503	-0.201	-0.077
S 1	0.649	-0.029	0.068	-0.097	-0.581

Table 3. Fukui indices for nucleophilic and electrophilic attacks for inhibitor DSD.

Table 4. Fukui indices for nucleophilic and electrophilic attacks for inhibitor DSDD.

АТОМ	$P_{N-1(r)}$	$P_{N+1(r)}$	$P_{N(r)}$	f_k^+	f_k^-
C1	0.093	0.118	0.124	-0.006	0.031
C2	-0.073	-0.023	-0.048	0.025	0.025
C3	-0.487	-0.413	-0.434	0.021	0.053
C4	-0.500	-0.437	-0.447	0.010	0.053
C5	0.378	0.214	0.426	-0.212	0.048
C6	-0.117	-0.049	-0.096	0.047	0.021
C7	-0.261	-0.251	-0.263	0.012	-0.002

ATOM	$P_{N-1(r)}$	$P_{N+1(r)}$	$\boldsymbol{P}_{N(r)}$	f_k^+	f_k^-
C8	-0.266	-0.235	-0.252	0.017	0.014
C9	-0.256	-0.241	-0.252	0.011	0.004
C10	-0.265	-0.249	-0.258	0.009	0.007
C11	-0.255	-0.253	-0.253	0.000	0.002
C12	-0.25	-0.254	-0.252	-0.002	-0.002
C13	-0.259	-0.261	-0.259	-0.002	0.000
C14	-0.256	-0.250	-0.254	0.004	0.002
C15	-0.242	-0.240	-0.241	0.001	0.001
C16	-0.253	-0.248	-0.251	0.003	0.002
C17	-0.447	-0.445	-0.446	0.001	0.001
N1	-0.560	-0.663	-0.595	-0.068	-0.035
01	-0.673	-0.677	-0.677	0.000	-0.004
O2	-0.631	-0.671	-0.666	-0.005	-0.035
O3	-0.426	-0.704	-0.503	-0.201	-0.077
S 1	0.647	-0.029	0.068	-0.097	-0.579

The site with utmost f_k^+ shows the most susceptible location to experience nucleophilic attack whereas site with utmost f_k^- reveals the most susceptible site where electrophilic attack may occur. Thus, from the results shown in Tables 2–4 locations for nucleophilic and electrophilic attacks were C6 (0.047) and O3 (0.170) for **DSO**, for **DSD** the highest value for f_k^+ was located on C6 (0.047), and the highest value for f_k^- was established on C5 with 0.099 while the greatest value for f_k^+ was positioned on C6 with 0.047 and the highest value for f_k^- is found on C3 and C4 with 0.053 each for the **DSDD** molecule.

3.3. QSAR Analysis

The developed QSAR model was observed to link the calculated descriptors from quantum chemical calculations via density functional theory on 2,3-dihydroxypropyl-sulfanyl derivative to the experimental % inhibition efficiency of the inhibitors. The developed model predicted the observed inhibition efficiency as shown in Table 5 using Equation 9. Also, the calculated correlation coefficient, adjusted R^2 and cross validation revealed the effectiveness of the developed model as shown in Table 6:

$$\% IE = 104.490 - 43.0000 (E_{LUMO})$$
(9)

	Observed %IE	Predicted %IE	residual
1	93.74	93.74	-0.00
2	93.24	93.31	-0.07
3	93.38	93.31	0.07

0.926

0.963

1

Conclusion

3

Many molecular descriptors such as E_{LUMO} , chemical hardness (η), E_{HOMO} , chemical potential (μ), and band gap were calculated using quantum chemical method via density Functional theory and B3LYP/6-31G* basis set. There was a fair correlation between selected descriptors (E_{LUMO} , Dipole moment) and %IE. It appeared that decreasing values of chemical Potential, Log *P*, Area, volume, Ovality and polarizability enhanced the corrosion inhibition efficiency. However, the QSAR model developed showed that E_{LUMO} was the predominant molecular descriptor that described the corrosion inhibition efficiency of these compounds. Thus, the predicted corrosion inhibition efficiency fitted with the observed %IE.

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