

Research Article

Designing Novel Quinoline Derivative as Corrosion Inhibitor for Aluminium in Hydrochloric Acid Solutions

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Abstract

In this research, novel quinoline derivative as aluminium corrosion inhibitor was designed by utilizing twenty three (23) molecules of quinoline derivatives tested each as corrosion inhibitors for the aluminium in HCl solution; experimentally through weight loss method, and theoretical investigations using quantitative structure activity relationship (QSAR). The inhibition efficiencies of the quinoline derivatives obtained from the weight loss shows that some quinoline derivatives such as 5-MeQ, 5-ClQ, 8-TMeQ, 6-ACQ and 7-OHQ inhibits the corrosion better than others as indicated by percentage inhibition efficiency (IE). Quantum chemical calculation indicated that the most popular parameters which play a prominent role are the eigenvalues of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), the HOMO-LUMO gap (ΔE), chemical hardness and softness and the number of electrons transferred from inhibitor molecule to the metal surface. Based on the several physicochemical descriptors and investigation of the adsorption of these molecules on the aluminium surface by the QSAR study of twenty three quinoline derivatives with the aid of material studio, a model was developed and validated. On the basis of the physicochemical parameters, predicted inhibition efficiency of 97.7% obtained using experimental inhibition efficiencies at 303K in 0.4M HCl and 0.2g/mol inhibitor concentration, and the correlation matrix from the QSAR study; 5-chloro,7-hydroxy-quinoline (5-Cl,7-OH-C₉H₅N) was designed and accepted as new efficient and effective quinoline derivative inhibitor for aluminium corrosion in HCl acid solution.

Keywords

Quinoline Derivatives, Aluminium, Corrosion, Qsar Study, Quantum Chemical, Inhibition Efficiency, Predicted

1. Introduction

Corrosion is the deterioration of metal by chemical attack or reaction with its environment. It is a constant and continuous problem. All metals and alloys are susceptible to corrosion

since no single material may be suitable for all applications [1]. It is impracticable to eliminate corrosion completely, prevention would be more practical and achievable than complete

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elimination. It is generally easier to understand why corrosion occur than how. Most metals exist in nature (in ores and minerals) as compounds such as oxide, sulphides, sulfates etc because these compounds represents their thermodynamically stable state [1]. The metals are extracted from these ores after expending lot of energy. Hence under that, the nature of the material is substantially changed (i.e by alloying or using inhibitors) the metal will have a natural tendency to revert back to its natural thermodynamically stable state. This is the basic reason for metallic corrosion. Corrosion can cause dangerous and costly damages to oil, gas and water pipelines, bridges, public buildings, vehicles, water and waste water systems and even home appliances. The effects of corrosion include large loss of products and resources, and ecological damages [2].

Corrosion of metals costs the United States excess of \$276 billion per year. This loss to the economy is more than the Gross National Product of many countries around the world. It has been estimated that 40% of U.S.A steel production goes to the replacement of corroded parts and products [3]. Analysis of oil pipeline failures in oil and gas industries in the Niger Delta area of Nigeria showed corrosion as one of the major causes of failure [3]. SPE (2008) stated in their report that Nigeria's oil and gas industry suffered greatly due to deterioration of essential metallic materials such as surfaces of metallic container, pipelines, plant parts etc between 2000 and 2004. The total pipeline breakage loss figure due to corrosion in 2004 alone was 396,000 metric tons (about four super tankers) while the financial losses were estimated to be ₦19.66 billions (US \$154.4). This menace of corrosion of metals in the oil, metallurgical and other industries has been widely acknowledged and several researches have been carried out on the protection of metals against corrosion. The results obtained revealed that one of the best methods involves the use of inhibitors since corrosion occurs due to the incompletely filled last orbital in the metal [4]. However, owing to stringent environmental regulations, organic compounds are preferred to inorganic compounds especially heavy metals derivatives, as corrosion inhibitors. Organic compounds containing hetero atoms such as N, S, P or O in conjugated or aromatic systems have been reported to be effective corrosion inhibitors [4]. The presence of polar functional groups (such as $-NH_2$ and $-OH$) as well as π -electrons facilitates the adsorption of the inhibitor on the surface of the metal [4].

Corrosion occurs with aluminium naturally as nature attempts to return metals to their original, stable, oxidized state. The degree and severity of corrosion that happens over time is a function of both the material and its operating environment. Aluminium corrosion can occur gradually over weeks, months, or even years [5]. With enough time, aluminium products can develop large holes due to corrosion. Scratching this oxide skin exposes bare metal, and the process begins again. It won't eat the metal away though, except under two conditions. First, if chlorides or sulphides are around they'll attack the aluminium oxide layer. Second, if conditions are tight you could ex-

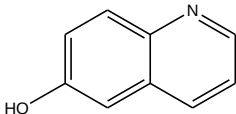
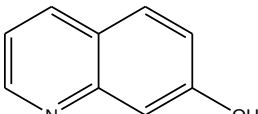
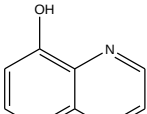
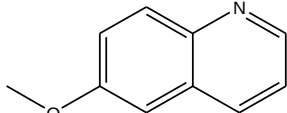
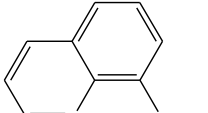
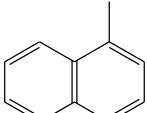
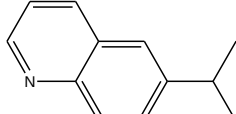
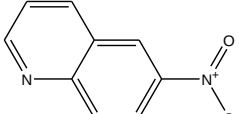
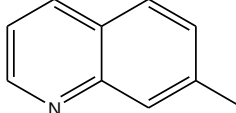
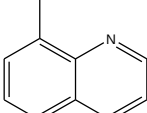
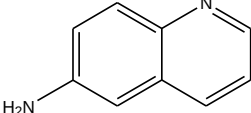
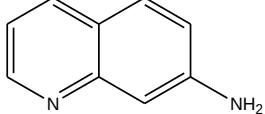
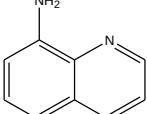
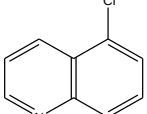
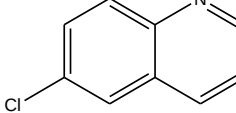
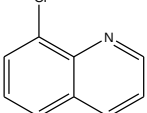
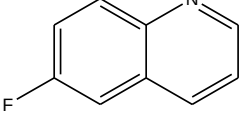
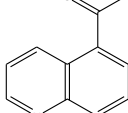
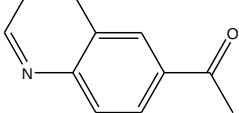
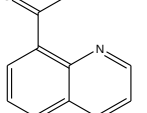
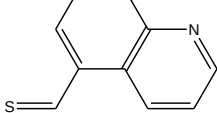
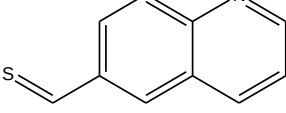
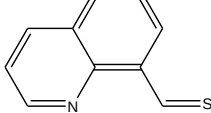
perience galvanic corrosion. This is an electrical effect experienced when dissimilar metals are brought close together in a conducting liquid [5]. For example, immerse brass and aluminium in seawater and electrons move from the aluminium to the brass. This can be a problem in boats where brass fittings are close to or even in contact with aluminium. (Fuel tanks are a prime example). Efforts have been made by many researchers to protect the integrity of the aluminium surfaces in an aggressive acid medium or other corrosive environment. The addition of inhibitors has been considered to be the most common approach to hinder the corrosion of aluminium. Thus, aluminium and its alloys are been extensively used for both domestic and industrial applications. To study the effect of temperature and corrodent concentration on the corrosion of aluminium in aggressive medium is of paramount important due to the fact that the stability of the oxide film is dependent upon the temperature and pH of the environment [6].

Many experimental methods and modern surface characterization tools have been created to evaluate and characterize the performance of corrosion inhibitors for metals and alloys [6]. These methodologies are often expensive, time consuming and tedious. Computational methods have already proven to be very useful in determining the inhibitors molecular structure and elucidating its electronic properties and reactivity. The use of computational chemistry such as density functional theory (DFT), molecular dynamic simulation (MD), Monte Carlo (MC) simulation and quantitative structure-activity relationship (QSAR) modelling has been applied to study the corrosion inhibition properties of organic molecules. Aromatic rings has mostly been regarded as the zones through which certain inhibitors can protect etching of metals [7].

Chemical attack on these metals leads to their deterioration (corrosion), which in turn leads material losses, as well as the accompanying economic losses. Since corrosion cannot be eliminated or avoided completely, it is important to at least manage or minimize the rate of corrosion using corrosion inhibitors (Organic inhibitors (ie quinolines) which are environmental friendly are preferred over inorganic inhibitors (e.g. chromates, dichromates, arsenates etc.) which are mostly toxic and hardly soluble salts [8]. So many organic corrosion inhibitors for aluminium have been designed and used, but still because of the importance of the metal aluminium a lot more effective and efficient corrosion inhibitors need to be developed [8].

The detail mechanism of the quinoline derivatives inhibition on aluminium metal in acid solution will be evaluated and established. Correlations between the potential of some quinoline derivatives as aluminium corrosion inhibitors in HCl and their structures had been assessed. This paved way in establishing molecular descriptors responsible for the inhibition process which will lead to the design of new efficient and effective quinoline derivative inhibitors for aluminium metal in acid solution. The following are the name and structures of each quinoline derivatives used in this research as shown in Table 1.

Table 1. Name and structure of the Quinoline derivatives used.

S/No	COMPOUND	S/No	COMPOUND	S/No	COMPOUND
1	 6-hydroxyquinoline	2	 7-hydroxyquinoline	3	 8-hydroxyquinoline
4	 6-methoxyquinoline	5	 8-methoxyquinoline	6	 5-methylquinoline
7	 6-isopropylquinoline	8	 6-nitroquinoline		
9	 7-methylquinoline	10	 8-methylquinoline	11	 6-aminoquinoline
12	 7-aminoquinoline	13	 8-aminoquinoline	14	 5-chloroquinoline
15	 6-chloroquinoline	16	 8-chloroquinoline	17	 6-fluoroquinoline
18	 5-acetylquinoline	19	 6-acetylquinoline	20	 8-acetylquinoline
21	 5-thiomethylquinoline	22	 6-thiomethylquinoline	23	 8-thiomethylquinoline

2. Methodology

In this study, experimental method was first carried out via weight loss to obtain the experimental inhibition efficiencies of all the twenty three (23) quinoline derivatives which was

used in the QSAR study to get the predicted inhibition efficiency for the newly designed inhibitor.

2.1. Weight Loss Method

In the weight loss experiment, rectangular aluminium specimens of area 4.0 x 3.0 cm (thickness = 0.15 cm), with small

hole of about 2 mm diameter just near one end of the specimen, have been used. The aluminium specimens were suspended by pyrex glass hooks to the depth below the surface of the corrosive solution (HCl) to prevent inclination of the aluminium coupon to the body of the container and ensure uniformity of interaction with the solution [9]. The volume of the solution for all the experiments was 100 cm³. Only one specimen was suspended in a pyrex glass beaker of 100 ml capacity. Experiments were performed in triplicate. The relative differences between triplicate experiments were found to be smaller than 5%, indicating good reproducibility. Initial weight of the test specimens were taken up with a digital balance. Then the specimens were immersed in the corrosion medium with and without different concentrations of the inhibitors. The solution contain either only a given concentration of the corrosive HCl without inhibitor or a given concentration of the corrosive HCl and inhibitor concentrations in an open beaker. The beaker was covered with a polyethylene material and tied with a rubber bung to prevent evaporation and then was inserted into a water bath maintained at certain temperature. Each coupon was withdrawn from the test solution after every hour using forceps, washed with hard brush under tap, rinsed with distilled water and then acetone, dried in air, weighed and recorded. It was then re-introduced back into the test solution for further analysis. The weight difference between the corroded and uncorroded coupon was calculated. The difference in weight for a period of 4 h was taken as total weight loss. The experiments were repeated at 313 and 323 K respectively [10].

From the weight loss results, the weight loss difference, degree of surface coverage (θ), inhibition efficiency (%IE) of the inhibitor and corrosion rates (CR in gh⁻¹cm⁻²) were calculated using Equations (1):

$$\% \text{ IE} = \left(1 - \frac{W_1}{W_2}\right) \times 100 \quad (1)$$

Where W_1 and W_2 are the weight losses (g) for aluminium in the presence and absence of the inhibitor in HCl solution, θ is the degree of surface coverage of the inhibitor, A is the area of the aluminium coupon (in cm²), t is the immersion time (in h) and ΔW ($W_i - W_f$) is the weight loss of aluminium coupon after 4 h.

2.2. QSAR Study

The materials and instruments used in this research include: aluminium, quinoline derivatives and Dell Computer Core i5 16G RAM of high resolution, install with Material studio Version 2017. The processes involved are too complex to model from first principles. The best way of using molecular modeling to help with the design of new and better corrosion inhibitors is to encapsulate knowledge about how existing inhibitors perform into a structure-activity relationship (SAR) and use this to predict the behaviour of new structures. The structures with the best predicted activity can then be used or further investigated [11].

Qsar Modeling Steps And New Compound Design

The structures of all the molecules were sketched and optimized through the Materials Studio software. The following molecular modeling stages were utilized using the material studio:

- 1) Begin by starting Materials Studio and creating a new project; New Project dialog was opened and Corrosion inhibitor was entered as the project name, there by clicking the OK button. The new project was created with *Corrosion inhibitor* listed in the Project Explorer. A new study table document was created by Selecting File/New from the bar to open the new Document dialog. Study table was selected and there by clicking the OK button. Renamed the study table Cl.std [12].
- 2) Imported and validated the structures and experimental data; The first step in validating the structures contained in the study table was to visually inspect them and to try to correlate the structural features present with the corrosion inhibition values provided. Double clicking on the structural Corrosion-1 in the Cl.std study table. This opens a study table Document Detail view. Select Window/ Tile vertically from the menu bar. This arranges the open documents in a way that enables you to see both the structure and the *Corrosion inhibition* column of the study table.
- 3) The structures were aligned in a table.
- 4) Molecular descriptors were calculated.
- 5) The initial data analysis was performed. Before building a correlation model, there is the need perform some elementary statistical analyses. Press the ESC key to deselect all the cells in the study table. down the CTRL key and click on the following headers in the study table: C, D, E, F, H, I, and J. Select Statistics | Initial Analysis | Correlation Matrix from the menu bar. This creates and displays the correlation matrix, CI - Correlation Matrix.xgd, of the data in the selected columns (Materials Studio 8, 2017).
- 6) The structure-activity relationship or model was built and validated.
- 7) Atom-based descriptors were added at different position on the quinoline molecule.
- 8) The New Model was Built and Validated.
- 9) A New candidate corrosion inhibitor was Created which is a derivative of the initial inhibitors. Clicking once in the new 3D Atomistic document to deselect everything and rotate the structure until the two hydrogens on the terminal amine group are visible. One of the two amine hydrogens was selected and click the Modify Elementar-row on the Sketch toolbar, choose Carbon from the dropdown list. The hydrogens were adjusted and the structure was cleaned. The new document was named as the Trial Inhibitor.std. Select Modules | Forcite | Calculation from the menu bar to open the Forcite Calculation dialog. On the Setup tab select Geometry Optimization from the Task dropdown list. On the Energy tab select

COMPASS from the Forcefield dropdown list. Click the Run button and closing the dialog. A new folder is created, Trial Inhibitor Forcite Geometry Optimization, and then the calculation. When it was completed, the results were downloaded into this folder (Materials Studio 8, 2017) [13].

- 10) The predicted corrosion inhibition efficiency of the new candidate was calculated.

The candidate was added to the study table by using the *Insert From...* option on the *Edit* menu, by copying and pasting the candidate structure. Make CI.std the active document. In the Project Explorer, right-click on Trial Inhibitor.xsd in the Trial Inhibitor, Forcite Geometry Optimization folder and select Insert Into from the shortcut menu. Right-click on the row heading cell for 20 and select Calculate from the shortcut menu. This calculates all of the descriptors and statistical models for the new inhibitor structure. Scroll to the right-hand side of the CI study table. The predicted inhibition efficiency

of the new trial structure is displayed. This have a higher inhibition value of around 15 or more (Materials Studio 8, 2017). The residual column contains an #N/A error as there is no experimental activity from which to calculate the residual. To get the best out of all the structures used as corrosion inhibitors for aluminium, all the substituent were tested at different positions on the quinoline core molecule. The one with highest activity was accepted and the others were discarded [14].

3. Results and Discussions

The Figure 1, presented here were based on the weight loss method used to study the variation in corrosion inhibition efficiency of the quinoline derivatives on the aluminium coupons in hydrochloric acids at varying temperatures. Variation of inhibitor mass and that of HCl (corrodent) concentrations at three different temperatures were considered.

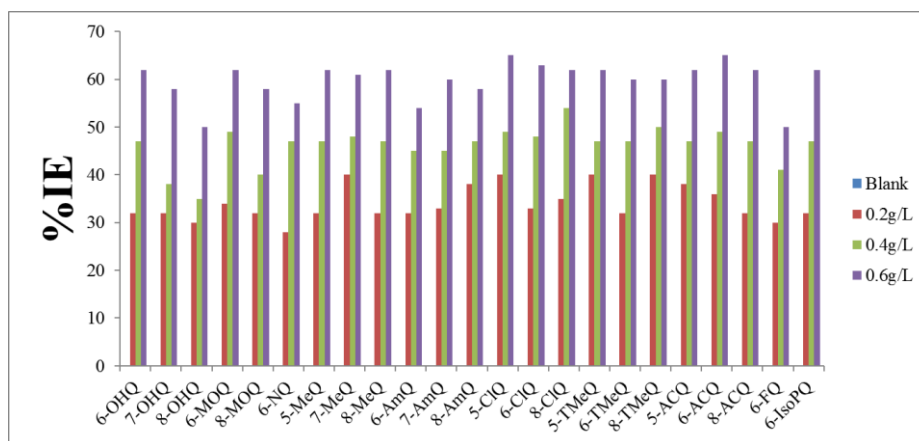


Figure 1. %IE for corrosion of aluminium in 0.4M HCl at 303K in varying inhibitors concentrations.

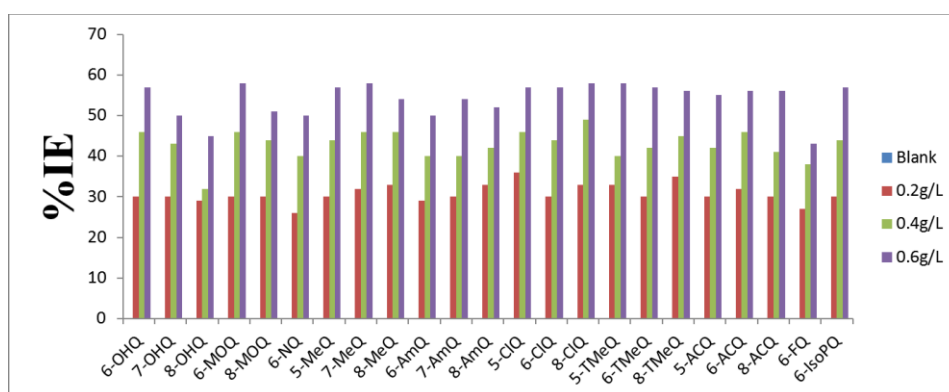


Figure 2. %IE for corrosion of aluminium in 0.4M HCl at 313K in varying inhibitors concentrations.

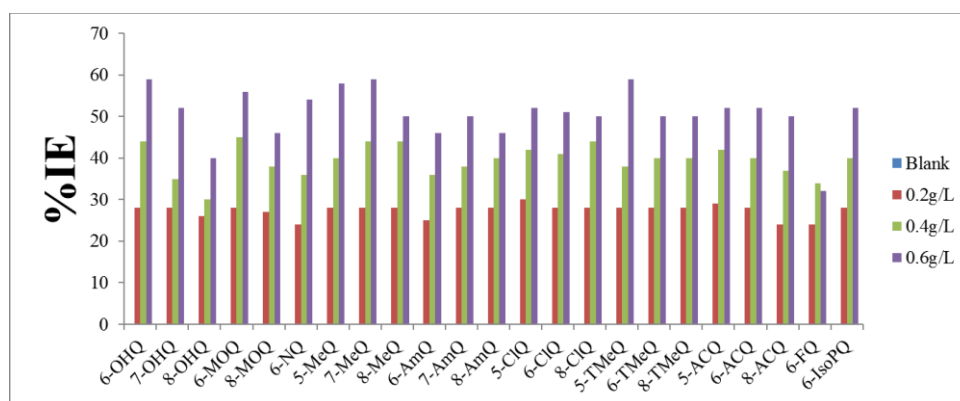


Figure 3. %IE for corrosion of aluminium in 0.4M HCl at 323K in varying inhibitors concentrations.

For clarity and in-depth observation, the inhibitors are grouped according to the type of substituent attached to the quinoline molecule. All substituents position on quinoline influences the performance on inhibition of aluminium corrosion and the effect can be observed from the Figures 1 to 3 through weight loss experiments. Comparatively inhibition efficiency obtained from the weight loss indicated the superiority in performance of some derivatives having the same substituent but different position on the core quinoline.

The corrosion inhibition performance profile of all the pairs for the anti-corrosion effect on aluminium via weight loss experiment shown in the Figures 1 to 3 indicates a progressive decrease in weight loss with increase in the inhibitors masses (g/L) at all temperatures for all the system concurrently under the same condition. The vertical height of the bars in the Figures 3, 1 is a function of the amount of weight lost by the aluminium in test for the blank and the inhibited case for all the system. This is in agreement with the fact that the presence of inhibitor molecule prevent the corrodent molecules (acid) from having full contact with the metal surface such that a barrier has been created in between which could be physically or chemically depending on the adsorption characteristics [14]. Another observable effect from the Figures 1 to 3 that the difference in corrosion inhibition efficiency among the pairs of molecules (hydroxyquinolines, methylquinolines, chloroquinolines, aminoquinolines, acetylquinolines and thiomethylquinolines) each pair with the same substituent and similar molecular weight. This occurred as a result of intramolecular activity/interaction which is suspected to take place more severely in those molecules with least inhibition performance comparatively. Some are more adsorbed on the metal surface than the others, and so regardless of the inhibitor dose applied [15]. This is the more reason why QSAR modelling becomes valid to design more effective inhibitor by selecting the best derivative and putting the substituent on the most better position for an improved corrosion inhibition efficiency [16].

Core and the Designed Quinoline Inhibitors From the QSAR

The following are the optimized structure of the core quinoline (Figure 4), extracted collection (Figure 5) after combining all the molecules prior to running of the model and the optimized structure of the designed quinoline inhibitors (Trial inhibitors).

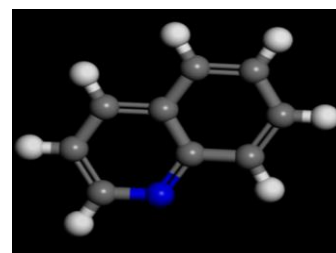


Figure 4. Optimized Core Quinoline.

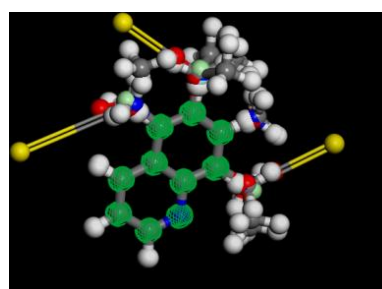


Figure 5. Collection of the inhibitor molecules.

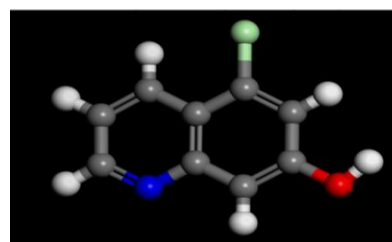


Figure 6. Trial Inhibitor 1.

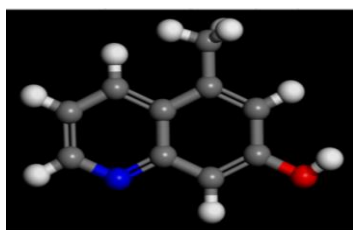


Figure 7. Trial Inhibitor 2.

The experimental inhibition efficiency obtained from the weight loss method was utilized to run the qsar computation through which the predicted corrosion inhibition efficiency was generated as shown in the [Tables 2 and 3](#) below at room temperature and at elevated temperature respectively.

Table 2. Experimental and theoretical corrosion inhibition Efficiency from QSAR study at 303k.

S/N	Molecule	Exp. %IE	Rotatable bond	H-bond (acceptor)	Pred. for C	Residual Value
1	5ClQ	70	0	1	71.83	-1.827
2	8ACQ	70	0	0	70.01	-0.010
3	6NQ	72	0	3	74.12	-2.119
4	8AMQ	73	0	2	73.01	-0.015
5	7MeQ	74	1	2	75.36	-1.364
6	8ClQ	74	1	2	73.02	0.981
7	8OHQ	74	0	2	73.13	0.873
8	6FQ	75	0	1	76.01	-1.011
9	8MOQ	75	1	2	74.90	0.105
10	Core	75	1	2	73.70	1.298
11	6MOQ	75	1	2	76.24	-1.244
12	6IpQ	76	0	1	76.32	-0.321
13	6OHQ	76	0	1	73.97	2.026
14	6AMQ	76	1	2	77.09	-1.085
15	8MeQ	76	1	2	75.78	0.224
16	6TMQ	76	0	2	76.93	-0.933
17	5ACQ	76	1	2	73.88	2.121
18	6ClQ	77	1	2	76.58	0.424
19	7OHQ	78	1	2	77.53	0.469
20	8TMQ	78	0	1	77.90	0.098
21	6ACQ	78	0	1	77.34	0.662
22	7AMQ	78	0	2	77.01	1.003
23	5MeQ	78	1	1	79.73	-1.724
24	5TMQ	85	1	2	83.62	1.371
25	Trial 1		2	3	97.77	#N/A
26	Trial 2		2	2	82.61	#N/A

The trial inhibitors (Trial 1 and Trial 2) were selected to be used in searching the right position of the substituent that can

give more better corrosion inhibition efficiency base on their appearance at the top with highest predicted inhibition efficiency after GFA (Genetic function Approximation).

Table 2 is the QSAR Study at 303K. The experimental inhibition efficiency at 303K is generally higher than that at 323K, ranging from 70% to 85%. The QSAR model performs better at this temperature, with smaller residuals (mostly below $\pm 2\%$) compared to 323K. Trial 1 and Trial 2 molecules have extremely high predicted inhibition efficiencies (97.77% and 82.61%). The best inhibitors (5TMQ, 5ClQ, 5MeQ, and 7OHQ) exhibit the highest experimental efficiencies. Some molecules (e.g., 6OHQ, 5ACQ) show positive residuals, meaning the model under-predicts their performance. Temperature effects are evident higher inhibition efficiency is observed at 303K compared to 323K, likely due to enhanced adsorption at lower temperatures [16-18]. The model performs better at 303K, indicating that temperature-dependent parameters should be considered in future models. Halogenation (e.g., 5ClQ, 8ClQ, 6FQ) continues to influence inhibition efficiency. More rotatable bonds and H-bond acceptors contribute positively to inhibition at low temperature. The QSAR model is more accurate at 303K, suggesting that corrosion inhibition mechanisms are temperature-dependent [19]. Most residual values are within a reasonable range, indicating a good predictive capability of the QSAR model at 303K [20].

The rotatable bond count, hydrogen bond acceptors, and molecular structure variations influence the predicted inhibition

efficiency as seen in Tables 2 and 3. Molecules with higher rotatable bond counts and more hydrogen bond acceptors generally show higher experimental inhibition efficiency. For example: 6OHQ (46%) and 6AMQ (47%) have one rotatable bond and two H-bond acceptors. 8TMQ (50%) and 6ACQ (50%) also have one rotatable bond and two H-bond acceptors, correlating with higher inhibition efficiency. Lower inhibition efficiencies (e.g., 5ClQ, 8ACQ, 6NQ with 32%) are associated with fewer hydrogen bond acceptors or limited molecular flexibility [21, 22].

For the model at lower temperature of 303K, Most molecules have 0 or 1 rotatable bond, suggesting that molecular flexibility does not significantly affect inhibition efficiency. Hydrogen Bond Acceptors: Molecules with 1 or 2 H-bond acceptors generally exhibit higher inhibition efficiency, reinforcing the role of hydrogen bonding in corrosion inhibition [23]. The high experimental inhibition efficiency observed with high predicted efficiency with a low residual error (1.37%), indicating a strong alignment between prediction and experiment. Molecules like 6OHQ (76%) and 5ACQ (76%) have slightly larger residual values (2.03% and 2.12%, respectively), suggesting minor deviations from the model [24]. The core structure (75%) shows good agreement between experimental and predicted values, implying that modifications around this structure influence inhibition performance [25].

Table 3. Experimental and theoretical corrosion inhibition Efficiency from QSAR study at 323k.

S/N	Molecule	Exp. %IE	Rotatable bond	H-bond (acceptor)	Pred. for C	Residual Value
1	5ClQ	32	1	2	43.71	-9.07
2	8ACQ	32	1	2	42.40	-9.07
3	6NQ	32	0	3	41.21	-6.01
4	8AMQ	33	0	1	41.14	-11.13
5	7MeQ	33	0	1	41.12	-11.13
6	8ClQ	33	0	2	41.12	-8.07
7	8OHQ	34	1	2	41.11	-7.07
8	6FQ	34	0	2	41.10	-7.07
9	8MoQ	36	1	2	41.06	-5.07
10	Core	40	0	1	40.15	-4.13
11	6MoQ	40	1	2	40.12	-1.07
12	6IpQ	43	1	1	40.10	-1.13
13	6OHQ	46	1	2	40.06	4.93
14	6AMQ	47	0	1	40.02	2.87
15	8MeQ	47	0	1	40.01	2.87
16	6TMQ	47	1	2	40.01	5.93

S/N	Molecule	Exp. %IE	Rotatable bond	H-bond (acceptor)	Pred. for C	Residual Value
17	5ACQ	47	1	2	40.01	5.93
18	6ClQ	47	0	2	40.00	5.93
19	7OHQ	48	1	2	39.07	6.93
20	8TMQ	50	1	2	39.03	8.93
21	6ACQ	50	1	2	38.27	8.93
22	7AMQ	52	0	1	38.12	7.87
23	5MeQ	52	0	1	37.87	7.90
24	5TMQ	52	0	2	34.13	10.9
25	Trial 1		1	3	58.07	#N/A
26	Trial 2		1	2	48.01	#N/A

Table 3 is the result of the experimental and Theoretical Corrosion Inhibition Efficiency from QSAR Study at elevated temperature of 323K. The table presents both experimental inhibition efficiency (%IE) and the predicted values derived from aQSAR (Quantitative Structure-Activity Relationship) model. There is a noticeable variation between experimental values and predicted values, as indicated by the residual values (difference between experimental and predicted values). The residual values vary from -11.13 to +10.9, suggesting that while the model performs well for certain molecules, it under-predicts or over-predicts inhibition efficiency in some cases [26]. In this case, there could be the need for model refinement for improvement of the model [26].

A. Model Equations For Run 1

The model equations for the first investigation (first run at room temperature) in the quantitative structure activity relationship (QSAR) model are shown below:

$$Y = -62.096649547 \times X_9 + 58.386422249 \quad (2)$$

$$Y = -48.769614102 \times X_{10} + 42.355922272 \quad (3)$$

$$Y = 14.651512911 \times X_{15} - 9.083974218 \times X_{37} - 77.06 \quad (4)$$

$$Y = -39.359006649 \times X_{10} + 7.008887052 \times X_{15} + 12.26 \quad (5)$$

$$Y = -47.697994252 \times X_9 + 6.508943566 \times X_{15} + 26.242 \quad (6)$$

$$Y = 282.496454889 \times X_{55} + 528.0737531 \times X_{57} - 126.2873 \quad (7)$$

$$Y = 14.732604846 \times X_{15} - 44.104156322 \times X_{38} - 75.32 \quad (8)$$

$$Y = 281.160652321 \times X_{55} + 485.798378054 \times X_{61} - 66.4605 \quad (9)$$

$$Y = -57.969500911 \times X_{10} + 7.209343179 \times X_{29} + 70.82 \quad (10)$$

$$Y = 14.758052977 \times X_{15} - 40.495683823 \times X_{40} - 73.907 \quad (11)$$

B. The Model Equations For Run 2

The model equations for the second investigation (second run at elevated temperature) in the quantitative structure activity relationship (QSAR) model are shown below:

$$Y = -32.224021892 \times X_8 + 0.202933686 \times X_{11} + 90.938 \quad (12)$$

$$Y = 0.188148130 \times X_{11} - 38.625138540 \times X_{26} + 149.0802 \quad (13)$$

$$Y = 0.193072449 \times X_{11} - 42.390929295 \times X_{31} + 191.157 \quad (14)$$

$$Y = 0.171676441 \times X_{11} + 86.792486369 \times X_{32} + 237.86 \quad (15)$$

$$Y = -41.001750698 \times X_{26} + 0.143474174 \times X_{45} + 141.79 \quad (16)$$

$$Y = -84.173579501 \times X_8 + 0.148980991 \times X_{45} + 53.387 \quad (17)$$

$$Y = 23.228977570 \times X_{31} + 0.141175022 \times X_{45} + 176.573 \quad (18)$$

$$Y = 0.188982165 \times X_{11} - 1.412368443 \times X_{43} + 55.22566 \quad (19)$$

$$Y = 0.187570977 \times X_{11} - 1.289288398 \times X_{44} + 74.578824 \quad (20)$$

$$Y = 0.157102321 \times X_{11} - 15.765333906 \times X_{13} + 57.5663 \quad (21)$$

The choice of the quantum chemical method used for energy minimization is expected to influence the molecular descriptors and, ultimately, the statistics of QSAR models [27]. The method of GFA technique was used to generate the ten QSAR models from which a model was selected and evaluated for each [28]. The chosen models were composed of many descriptors for the two runs respectively. The model was ran multiple times in order to accommodate the influence of temperature and other factors that may likely affect the performance of model [29]. The first one was ran with the experimental inhibition efficiency obtained at 323k (elevated tem-

perature) and the second one was ran using experimental inhibition efficiency at 303k (room temperature).

C. Model Accuracy and Performance

The QSAR model's predictive performance varies across different molecules. Some molecules, like 6OHQ, 6AMQ, and 8TMQ, have positive residual values, meaning the model underestimates their inhibition efficiency. Other molecules, like 8AMQ and 7MeQ, have large negative residual values, indicating an overestimation by the model [30]. The average residual value indicates that the model tends to predict lower than actual efficiency for certain inhibitors. Unlike in the second run (at elevated temperature), at low temperature the situation is quite different. There is low residual values across most molecules for the model at 303K demonstrated that the QSAR model effectively predicts corrosion inhibition efficiency [31].

D. Model Reliability

The QSAR model provides a useful predictive tool for corrosion inhibition efficiency, but it has limitations in accuracy

for certain molecules. Refinement of the model, possibly by incorporating additional molecular descriptors, could enhance predictive accuracy [32]. There is structural Influence on Corrosion Inhibition in some of the quinolin derivatives molecules used here. Molecules with higher flexibility (rotatable bonds) and stronger interactions (hydrogen bond acceptors) tend to show higher inhibition efficiency. Functional groups like -OH, -NH₂, and halogens (Cl, F, Br) may contribute to stronger adsorption on the metal surface, improving inhibition. 6OHQ, 6AMQ, 8TMQ, 6ACQ, 5CIQ and 7AMQ exhibit high inhibition efficiency ($\geq 47\%$), making them promising candidates for corrosion protection applications. The performance of 5MeQ, 5TMQ, and 7OHQ also suggests they could be further optimized for better inhibition performance [32]. This study confirms the effectiveness of QSAR modeling for predicting corrosion inhibition efficiencies but highlights the need for further refinement and validation for enhanced accuracy [32].

	A	B	C	D	E	F	G	H
		C : Corrosion inhibition	D : Rotatable bonds (Fast Descriptors)	E : Hydrogen bond donor (Fast)	F : Hydrogen bond acceptor (Fast)	H : AlogP (Fast Descriptors)	I : AlogP98 (Fast Descriptors)	J : Molecular refractivity (Fast Descriptors)
1	C : Corrosion inhibition	1	-0.33920300	-0.18601000	-0.33920300	-0.33298900	0.35393600	-0.34693200
2	D : Rotatable bonds (Fast Descriptors)	0.32273000	1	0.75000000	1	0.79795300	-0.93671200	0.99618600
3	E : Hydrogen bond donor (Fast Descriptors)	-0.02159440	0.75000000	1	0.75000000	0.19980300	-0.47096300	0.68942200
4	F : Hydrogen bond acceptor (Fast Descriptors)	0.13500500	1	0.75000000	1	0.79795300	-0.93671200	0.99618600
5	H : AlogP (Fast Descriptors)	0.19030300	0.79795300	0.19980300	0.79795300	1	-0.95846500	0.84750200
6	I : AlogP98 (Fast Descriptors)	-0.39513500	-0.93671200	-0.47096300	-0.93671200	-0.95846500	1	-0.96368800
7	J : Molecular refractivity (Fast Descriptors)	0.01367320	0.99618600	0.68942200	0.99618600	0.84750200	-0.96368800	1

Figure 8. Correlation matrix for Run 1.

	A	B	C	D	E	F	G	H
		C : Corrosion inhibition	D : Rotatable bonds (Fast Descriptors)	E : Hydrogen bond donor (Fast)	F : Hydrogen bond acceptor (Fast)	H : AlogP (Fast Descriptors)	I : AlogP98 (Fast Descriptors)	J : Molecular refractivity (Fast Descriptors)
1	C : Corrosion inhibition	1	0.01684890	0.11600200	-0.22208200	0.02433270	0.04310110	0.07524070
2	D : Rotatable bonds (Fast Descriptors)	0.01684890	1	-0.17960500	0.38691200	-0.13137600	0.02550760	0.52314000
3	E : Hydrogen bond donor (Fast Descriptors)	0.11600200	-0.17960500	1	-0.37525300	-0.60037400	-0.72553900	-0.35037200
4	F : Hydrogen bond acceptor (Fast Descriptors)	-0.22208200	0.38691200	-0.37525300	1	-0.05468770	0.05048310	0.17513500
5	H : AlogP (Fast Descriptors)	0.02433270	-0.13137600	-0.60037400	-0.05468770	1	0.96409900	0.23800700
6	I : AlogP98 (Fast Descriptors)	0.04310110	0.02550760	-0.72553900	0.05048310	0.96409900	1	0.40312700
7	J : Molecular refractivity (Fast Descriptors)	0.07524070	0.52314000	-0.35037200	0.17513500	0.23800700	0.40312700	1

Figure 9. Correlation matrix for Run 2.

Figure 8 is the correlation matrix of the first model (run 1) at 303K. It clearly shown an even distribution and adequate fit of the model. Figure 9 is the correlation matrix of the second model at 323K (run 2). It shows evidently that the model did not fit well and strong need for model refinement due to the effect of high temperature [33].

The low residual values across most molecules for the

model at 303K (run 1) demonstrate that the QSAR model effectively predicts corrosion inhibition efficiency. The model is well-calibrated, but a few molecules deviate slightly, suggesting that additional parameters (e.g., solubility, electronic properties) could refine the predictions further. The QSAR model at 303K (Run 1) provides a reliable prediction of corrosion inhibition efficiency with minor deviations. Hydrogen bonding and molecular flexibility influence efficiency, but the

core structure remains a key determinant. The experimental and theoretical values align well, validating the robustness of the QSAR approach in corrosion inhibition studies [33].

E. Genetic Function Approximation (GFA)

Table 4 is the Genetic Function Approximation for Run 1

(at 303K), Values range from 5.80 to 7.91, which are relatively low compared to Run 1 (Table 2), indicating an improved model fit [33]. R^2 -values range from 0.69 to 0.99, indicating a generally good model fit. The highest R^2 (0.990) suggests that one of the models explains almost all variance in the data [33].

Table 4. Genetic function Approximation for Run 1.

		1	2	3	4	5	6	7	8	9	10
1	Friedman LOF	65.05	67.03	67.15	67.42	67.50	67.59	67.59	67.658	67.72	67.78
2	R-squared	0.44	0.820	0.919	0.415	0.813	0.712	0.612	0.8111	0.401	0.954
3	Adjusted R-squared	0.06	-0.02	-0.03	-0.03	-0.03	-0.03	-0.03	-0.03	-0.04	-0.04
4	Cross validated R-squared	-0.1	-0.12	-0.16	-0.15	-0.22	-0.17	-0.12	-0.18	-0.18	-0.17
5	Significant Regression	Yes	Yes	Yes	No	Yes	Yes	Yes	Yes	Yes	Yes
6	Significance-of-regression F-value	1.141	0.455	0.416	0.326	0.300	0.272	0.272	0.249	0.228	0.210
7	Critical SOR F-value (95%)	4.303	4.303	4.303	4.303	4.303	4.303	4.303	4.303	4.303	4.303
8	Replicate points	0	0	0	0	0	0	0	0	0	0
9	Computed experimental error	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
10	Lack-of-fit points	22	22	22	22	22	22	22	22	22	22
11	Min expt. error for non-significant LOF (95%)	6.08	6.17	6.18	6.19	6.19	6.20	6.20	6.20	6.20	6.21

However, some models have R^2 around 0.69 - 0.79, which suggests moderate performance. Unlike Run 2, adjusted R^2 values are positive and range from 0.44 to 0.80, indicating that the models avoided over-fitting to some extent [33]. Equations 2 and 3 have higher adjusted R^2 values (~0.79 - 0.80), meaning they provide a balance between fit and complexity. There is significant variation, with values ranging from 0.67 to -5.20. Some model equations (e.g., (14), (15), and (19)) have very low or negative cross-validated R^2 values, indicating poor

generalization. However, some models (2) and (8) have positive cross-validated R^2 (~0.67, 0.401), suggesting better predictive performance. All models show statistically significant regression [33]. The F-values (9.02 to 19.3) are significantly higher than the critical F-value (2.79 - 4.60), confirming model reliability. Values range between 18 and 21, which is slightly lower than Run 2. The minimum experimental error for non-significant LOF (95%) is 1.07 - 1.83, meaning that the models have relatively low error [33].

Table 5. Genetic function Approximation for Run 2.

	Equation	1	2	3	4	5	6	7	8	9	10
1	Friedman LOF	5.80	5.95	7.21	7.55	7.69	7.79	7.81	7.85	7.85	7.91
2	R-squared	0.89	0.94	0.98	0.79	0.95	0.69	0.96	0.975	0.72	0.990
3	Adjusted R-squared	0.79	0.80	0.74	0.63	0.62	0.63	0.63	0.711	0.51	0.625
4	Cross validated R-squared	0.67	0.12	2.82	3.18	0.05	1.42	0.401	-5.20	0.025	1.75
5	Significant Regression	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

	Equation	1	2	3	4	5	6	7	8	9	10
6	Significance-of-regression F-value	19.3	19.2	9.88	9.65	9.35	10.82	10.81	9.02	9.02	10.59
7	Critical SOR F-value (95%)	2.79	2.794	4.608	3.257	3.257	2.94	2.94	3.257	3.25	2.945
8	Replicate points	0	0	0	0	0	0	0	0	0	0
9	Computed experimental error	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	Lack-of-fit points	23	18	21	20	20	22	19	20	20	22
11	Min expt. error for non-significant LOF (95%)	1.07	1.08	1.83	1.66	1.67	1.46	1.46	1.690	1.69	1.47

The Table 5 shows R^2 values range from 0.40 to 0.954, suggesting that the models have varying degrees of predictability, with Run 10 showing the highest fit ($R^2 = 0.954$) and Run 9 the lowest ($R^2 = 0.410$). The Adjusted R^2 values are negative in the second model at elevated temperature (run 2), which indicates that some models might have over-fitting issues or include non-significant variables. The Cross-validated R^2 values are negative (ranging from -0.12 to -0.27), meaning the models do not generalize well to new data and may not be reliable for prediction at the elevated temperature [33, 34]. This suggests that additional descriptor selection and refinement of model parameters are needed. The Significance-of-regression F-value is lower than the critical SOR F-value (4.303), indicating that some regression models may not be statistically significant. The lack-of-fit (LOF) points are high (22 for all runs), implying that the models do not adequately explain the variability in experimental data [34]. The computed experimental error is 0, meaning the model strictly relies on the available dataset without accounting for experimental variations. A minimum experimental error for non-significant LOF (95%) is between 6.08 and 6.21, which suggests that the models need improvement to reduce systematic errors. For this model in which the experimental inhibition efficiency used are taken at elevated temperature, may be highly affected by the temperature which necessitate model refinement if the model is to be acceptable [34]. The lower Friedman LOF values and higher R^2 values indicated that Run 1 (modelling at low temperature) performed better than Run 2 (at elevated temperature). The positive adjusted R^2 values suggest that these models are less prone to over-fitting compared to Run 1. Some models (Equations (2), (8), and (11)) have moderate cross-validated R^2 values, meaning they perform better for prediction [34]. The Best Models: Equations (2), (3), and (8) appear to be the most balanced, with high R^2 , adjusted R^2 , and positive cross-validation R^2 values [34]. These models should be prioritized for corrosion inhibition predictions. Run 1 (at low temperature) performed better than Run 2 (at elevated

temperature), showing lower LOF values and improved adjusted R^2 values [35].

F. Validation of The Models

In validation matrix, an acceptable QSAR model shall have an R -square value at least 0.6, R^2_{adj} not less than 0.5, Q^2_{cv} not greater than 0.3 and R^2 for external test set not less than 0.60 [36]. However, at 323K for the first model (run 2), the certain criteria were not fully aligned, and the model is considered partially accepted. Interestingly as reported in Tables 1, 3 and 5 respectively for the first run at 303K, the various parameters were predicted to satisfy the criteria specified by the thresholds for an acceptable QSAR model. In addition, the built models particularly equation (2), (3) and (8) (ME2, ME3 and ME8) showed a significant regression with the number of test set of compounds being very high [37]. Therefore the built models using experimental inhibition efficiency obtained at 303K were found to excellently satisfy the requirement for a reliable QSAR model [37].

4. Conclusion

After the successful investigation of quinoline derivatives as corrosion inhibitors for aluminium in HCl, both experimentally through weight loss as well as theoretically by quantum chemical calculations; the corrosion inhibition efficiency of a novel quinoline derivative (5-chloro,7-hydroxy-quinoline) was found to be approximately 98% at 303K and 58% at 323K which is more than the inhibition efficiency of the core quinoline of 74% at 303K and 40% at 323K respectively on the same metal under the same conditions.

On the basis of the physicochemical parameters, predicted inhibition efficiency of 97.7% obtained using experimental inhibition efficiencies at 303K in 0.4M HCl and 0.2g/mol inhibitor concentration, and the correlation matrix from the QSAR study; 5-chloro,7-hydroxy-quinoline (5-Cl,7-OH-Q) is designed and accepted as new efficient and effective quinoline derivative inhibitor for aluminium corrosion in acid me-

dium. The results showed that all the experimental and computational methods used exhibited good correlation for the parameters studied. The designed model successfully correlates electronic parameters with chemical reactivity and validates these findings through statistical analysis. It provides a robust theoretical framework for predicting the behavior of quinoline derivatives in the corrosion inhibition applications.

Abbreviations

DFT	Density Functional Theory
MD	Molecular Dynamic
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
E _{HOMO}	Energy of Highest Occupied Molecular Orbital
E _{LUMO}	Energy of Lowest Unoccupied Molecular Orbital

Conflicts of Interest

The authors declare no conflicts of interest.

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