Nigerian Research Journal of Chemical Sciences (ISSN: 2682-6054)
Volume 15, Issue 1, 2026

Utilization of *Tectona grandis Dye Extract* as Strong Inhibitor for Mild Steel Corrosion in Acidic Environment: A Computational Approach to Corrosion Inhibitor Design

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Accepted: *August 3, 2026* **Published Online***: August 7, 2026*

ABSTRACT

The aim of this study was to relate the structure of the *Tectona grandis* dye extract to their corrosion-inhibition. In this study the ability of *Tectona grandis* dye extract to inhibit mild steel corrosion in 1 M hydrochloric acid was investigated by using weight-loss experiments with quantum chemical calculations. Increasing the extract concentration improved inhibition efficiency, and computational results identified quercetin as the most active inhibitory component. The agreement between the theoretical and experimental results supports quantum chemistry as a useful approach for studying metal corrosion protection.

KEY WORDS: Corrosion, mild steel, hydrochloric acid, quercetin corrosion rate

INTRODUCTION

Corrosion of metal surfaces remains a persistent problem in industry and materials science, and the use of inhibitors is the most common way to control it. Corrosion inhibitors work by adsorbing onto the metal surface and forming a barrier against the surrounding corrosive medium. Molecules containing nitrogen, oxygen, or sulfur atoms, particularly those arranged in ring or chain structures, have repeatedly been shown to act as effective inhibitors [1]. Plant extracts are a valuable alternative source of inhibitors, and several studies have confirmed their inhibitory activity against corrosion [2-4]. Quantum chemical calculations have also become a standard tool for probing the mechanisms behind corrosion inhibition [5, 6], linking the molecular structure of organic inhibitors to their performance and informing the design of new candidates [7, 8]. Teak (*Tectona grandis*) contains tannins, alkaloids, flavonoids, anthraquinones, and naphthoquinones compounds bearing oxygen and nitrogen atoms and functional groups capable of hindering corrosion [9]. *Tectona*

grandis leaf extract has already been tested against mild steel corrosion in acidic media [10-12], but data linking its inhibition efficiency to quantum chemical predictions are still limited.

The aim of this study is to relate the structure of the *Tectona grandis* dye extract to their corrosion-inhibition and the specific objective of this research is to predict the inhibitors active compounds using the computational techniques**.**

MATERIALS AND METHOD

Sample collection

The leaves of *Tectona grandis* were collected within the premises of Holy Saviour Secondary School, Ile Oluji, in Ondo State, Nigeria, and authenticated at the Biology Unit, Department of Science Laboratory Technology, Federal Polytechnic Ile Oluji, Ondo State.

Extraction of *Tectona grandis Dye*

Tectona grandis leaves were washed to remove impurities and shade-dried for three weeks. The dried leaves were pulverized and sieved to a uniform particle size. For dye extraction, 500 g of the powder was soaked in 2 L of 50% ethanol for 3 days, and the mixture was then filtered to separate the liquid extract from the leaf residue. The extract was concentrated and stored in a refrigerator until use.

Phytochemical analysis

Established methods were employed to identify the phytochemical constituents present in the TG dye extract [13]**.**

Test for alkaloids

A 0.5 g sample of the powdered material was extracted with dilute hydrochloric acid. The resulting extract was then treated with Mayer's and Dragendorff's reagents. The formation of a precipitate in either test indicated the possible presence of alkaloids.

Test for tannins

A 0.5 g sample of the dried powdered material was boiled in 20 mL of water, and the resulting solution was filtered. The addition of ferric chloride produced a brownish-green or blue-black colour, indicating the presence of tannins.

Test for saponins.

A portion of the 2 g of powdered material was boiled in 20 mL of distilled water, and the resulting solution was filtered. A 10 mL of the filtrate was then shaken vigorously to produce a foam. The foam's stability was observed, and a small amount of olive oil was added. The mixture was shaken again to determine if a stable emulsion had formed, indicating the possible presence of saponins.

Test for flavonoids

The powdered sample was extracted with 10 mL of ethyl acetate using heat from the stem bath for 3 min. A 4 mL of the resulting extract was then treated with 1 mL of a dilute ammonia solution. A yellow colour indicated the possible presence of flavonoids.

Test for cardiac glycosides

A 5 mL of the extract was reacted with a mixture of 2 mL of glacial acetic acid and ferric chloride. A 1 mL of concentrated sulphuric acid was then carefully added. The formation of a brown ring at the interface suggests the presence of a deoxy sugar, indicative of cardenolides. Additionally, a violet ring might appear below, and a green ring could gradually develop within the acetic acid layer.

Test for anthraquinone

Few drops of magnesium acetate solution were added to 1 mL of the extract; the formation of pink colour showed the presence of anthraquinone.

Test for phenol

A few drops of ferric chloride solution were added to 2 mL of the extract in a watch glass; the appearance of bluish green colour indicated the presence of phenol.

Weight-loss measurement

Pre-weighed coupons were immersed in the HCl solution for 3 hours at 303 K, with and without varying concentrations of *Tectona grandis* crude extract. After immersion, the coupons were removed, washed in NaOH solution, rinsed with distilled water and acetone, dried, and reweighed to determine the mass loss. Average weight-loss values were used in Equations (1), (2), and (3), following the methods outlined by Olasehinde et al. [13] to calculate corrosion rate (CR).

$$C.R = \frac{\Delta w}{At} \quad (1)$$

Where Δw = change in weight in g

A = Area in cm^2

t = Time in hour

$$\% I.E = I - \frac{\Delta w_1}{\Delta w_2} \times 100 \quad (2)$$

Where Δw_1 and Δw_2 are uninhibited and inhibited weight loss measurements.

$$\Theta = 1 - \frac{\Delta w_1}{\Delta w_2} \quad (3)$$

The procedure was repeated at temperature values of 313 K,323 K, and 323 K.

GC-MS and HPLC Analysis

The TG dye extract was analyzed by gas chromatography-mass spectrometry to identify and quantify its components, and further characterized by High-Performance Liquid Chromatography (HPLC)

GC-MS analysis

Sample extracts were analysed with GC-MS analysis using an Agilent Technologies 8860A (GC) model interfaced with a mass selective detector (Model: 5975C (MSD). The ion source temperature was 250 ^oC, and the electron ionization was conducted at 70 volts. A HP-5 column (30 mm x 0.25 mm x 0.320 μm) was filled with 99% pure helium gas as a carrier gas. The oven was preheated to 80 °C, held for one minute, and then ramped up to 240 °C at a rate of 10 °C per minute, kept for five minutes. A 1μL sample was injected.

HPLC Analysis

An Agilent 1260 HPLC with a variable-wavelength detector was used for this study. An Agilent Poros Hell 120EC C18 4um, 150 x 4.6 mm column was utilized. 280 nm was the measuring wavelength, and the mobile phase composition was 0.1% formic acid: 0.2% formic acid in methanol gradient.

Quantum chemical calculations

The Hartree-Fock Density Functional Theory (HF-DFT) with the Becke 3 Lee Yang Parr (B3LYP) method and a 6-31G* basis set within the Spartan '14 VI.1.4 program software were used to perform quantum chemical studies on the corrosion inhibitors.

RESULTS AND DISCUSSION

Investigation of the phytochemical profile

Phytochemical screening of the TG dye extract detected alkaloids, flavonoids, saponins, phenols, anthraquinones, and tannins. As shown in Table 1, saponins, tannins, and alkaloids have been identified as active constituents in some green inhibitors [9].

Table 1: Phytochemical profile of TG dye extract

Parameter	Observation
Alkaloids	+++
Flavonoids	++
Saponins	++
Cardiac Glycosides	++
Anthraquinones	++
Tannins	++
Phenols	+++

Corrosion Rates

Figure 1 shows the corrosion rates in the presence and absence of *Tectona grandis* dye. Corrosion rate rose with increasing temperature, most likely because higher temperatures degrade the protective layer on the metal surface. Higher temperatures also speed up hydrogen gas evolution, which promotes further corrosion [14]. In contrast, the corrosion rate fell as TG dye concentration increased, confirming that the dye is effective at slowing corrosion.

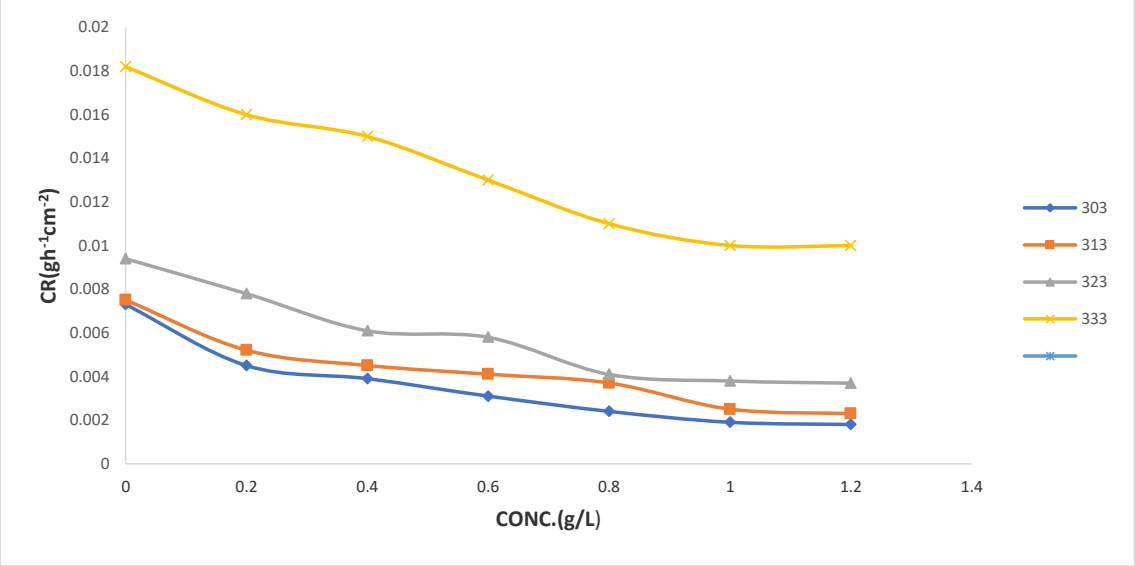

Figure 1: Corrosion rate in the presence and absence of *Tectona grandis* dye extract

Inhibition efficiency

Figure 2 shows the percentage inhibition efficiency (IE). IE increased with rising concentrations of *Tectona grandis* dye, consistent with earlier findings [15], suggesting that still higher concentrations could give further inhibition.

The inhibitory action of the TG dye extract is likely due to natural compounds such as tannins, flavonoids, polyphenols, and alkaloids, which contain nitrogen, sulfur, and oxygen atoms capable of bonding with iron on the metal surface. This bonding forms a passivation layer that limits contact between corrosive ions and the metal.

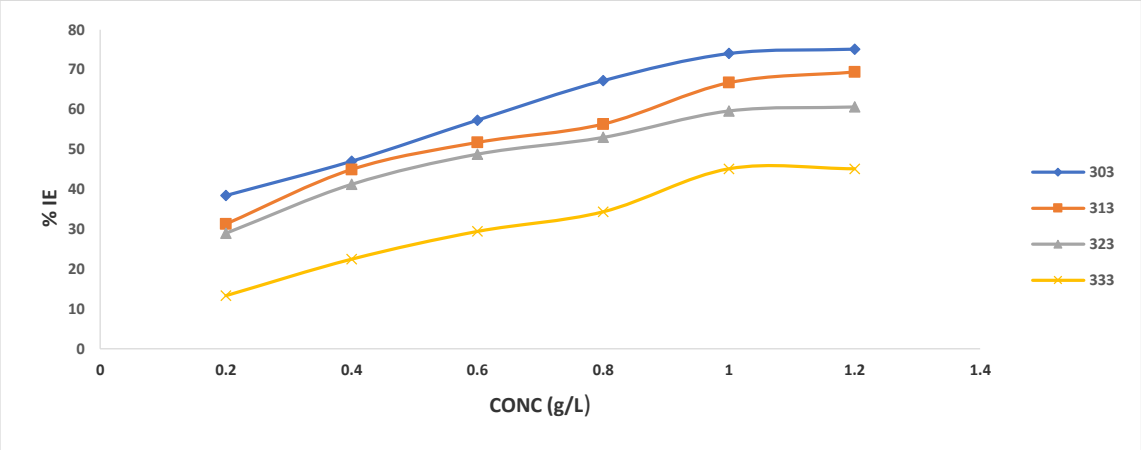

Figure 2: Inhibition efficiency of *Tectona grandis* dye extract

Tables 2 and 3 show the results of GCMS and HPLC analysis of *Tectona grandis* extract respectively.

Table 2: GC-MS analysis for *Tectona grandis* extract

Pk NO	RT	Area%	Library/ID	Ref NO	CAS NO	Qual
1	4.855	1.66	Furfural	2766	000098-01-1	86
2	5.027	1.10	3,5-Dimethylpyrazole	2782	000067-51-6	78
3	5.656	1.10	2-Furanmethanol	3127	000098-00-0	76
4	7.882	32.99	Phenol	2619	000108-95-2	91
5	8.637	1.37	Ethyl2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate	103910	1000373-80-3	50
6	8.883	1.02	trans-Linalooloxide(furanoid)	39617	034995-77-2	47
7	9.238	1.54	2-Furanmethanol,5ethenyl tetrahydro-.alpha.,.alpha.,5-tri methyl-, cis-	39796	005989-33-3	91
8	9.358	1.04	p-Cresol	5461	000106-44-5	95
9	9.513	2.70	Phenol, 2-methoxy-	10619	000090-05-1	87
10	11.584	2.16	Benzofuran, 2,3-dihydro-	9568	000496-16-2	70
11	13.364	2.05	Phenol, 2,6-dimethoxy-	28298	000091-10-1	97
12	13.730	1.88	1-Propanone,1-(1,3-benzo dioxol-5-yl)-3-(1piperidinyl)-	121909	30418-51-0	38
13	14.119	3.39	Ethanone,1-(3hydroxy phenyl)-	16724	000121-71-1	97
14	14.502	16.38	Pyrazole-1-methanol	3077	001120-82-7	47
15	16.682	2.07	7-Octen-2-ol,2-methyl-6-methylene	27653	000543-39-5	38
16	16.883	2.35	1,4-Benzenediol,2,5-dimethyl	17786	000615-90-7	38
17	17.066	3.13	Cyclooctene, 1,2-dimethyl-	17305	054299-96-6	30

18	17.312	1.54	Hydrazinium, 2-cyano-1,1,1-trimethyl-,hydroxide,inner salt	3524	035468-56-5	38
19	17.833	5.59	Decahydro-8a-ethyl-1,1,4a,6 tetramethyl naphthalene	85949	1000100-23-6	47
20	18.948	1.08	Phenol, 3-(dimethylamino)-	17158	000099-07-0	64
21	19.852	4.36	Hexadecanoic acid, methyl ester	130822	000112-39-0	98
22	21.472	3.67	9,12-Octadecadienoic acid, methyl ester	153873	002462-85-3	99
23	21.529	4.78	9-Octadecenoic acid (Z)-, methyl ester	155750	000112-62-9	99
24	27.572	1.04	1-Bromo-11-iodoundecane	212906	139123-69-6	46

Table 3: HPLC Analysis for *Tectona grandis dye* extract

S/N	Retention Time [min]	Compound Name	Concentration mg/L
1	6.922	Catechin (Hydrate)	0.216
2	12.291	Naringin	6.151
3	16.188	Myricetin	0.001
4	18.667	Baicalin	8.170
5	21.926	Quercetin	2.010
6	25.586	Kaempferol	0.028
7	28.507	Baicalein	0.012

GC-MS identified 24 bioactive compounds in the TG dye extract, with 9-octadecenoic acid (Z) methyl ester the most abundant. HPLC identified 14 bioactive compounds, dominated by baicalin,

naringin, and quercetin. Quercetin was the one compound detected by both techniques, consistent with previous reports [16-18].

Quantum Chemical Studies

DFT/B3LYP calculations give access to molecular properties including HOMO and LUMO energies, the energy gap, ionization potential, electron affinity, dipole moment, global hardness, and softness; the resulting values are listed in Table 4.

An effective corrosion inhibitor needs to do two things: draw electrons away from the metal surface and donate its own electrons into the metal's vacant d-orbitals to form bonds. Both abilities are governed by the inhibitor's frontier molecular orbitals, the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) [19]. LUMO reflects a molecule's capacity to accept electrons from the metal, while the electron-rich HOMO governs electron donation. Optimized structures of the TG dye components are shown in Figures 3 and 4. In the orbital diagrams, blue regions mark high electron density and red regions mark low density. Figures 3(b and c) and 4(b and c) show these orbitals for 9-octadecenoic acid (Z) methyl ester and quercetin, the two compounds found in the TG dye extract. In both molecules the HOMO and LUMO are distributed over the oxygen atoms of the hydroxyl and carboxylic groups, the double-bonded carbons, and the aromatic rings, marking these as the likely sites of interaction with the metal surface, since electrophiles preferentially attach at the same regions [17]. Molecules with a higher HOMO energy give up electrons more readily and inhibit corrosion more strongly. Comparing EHOMO values, quercetin is predicted to donate electrons more easily than 9-octadecenoic acid (Z) methyl ester, and computational results accordingly suggest quercetin has the stronger inhibition properties of the two.

A lower LUMO energy (ELUMO) means a greater tendency to accept electrons. Quercetin has the lowest ELUMO of the two compounds, making it the better electron acceptor, while 9-octadecenoic acid (Z) methyl ester has the highest. As a whole, the electron-donating and accepting properties of such compounds help account for the protection provided by the TG dye extract to the mild steel surface, supporting the results concerning weight loss presented above.

Moreover, the energy gap between the HOMO and LUMO states (ΔE) is also essential for determining the adsorption capacity of the inhibitor on the metal surface – the smaller the energy

gap is, the easier electron donation and accepting and, thus, stronger inhibition is expected, while the higher the energy gap is, the more stable the compound and, therefore, less reactive. It is known that the energy gap of quercetin is lower than that of 9-octadecenoic acid (Z) methyl ester, confirming the former's greater potential as an inhibitor.

Dipole moment (μ) is considered to be an indicator of charge distribution and can influence adsorption both directly and indirectly. Some researches found the higher dipole moment value to correspond to higher adsorption [20]. while others proved the contrary [21]. In the present study, the dipole moments of quercetin and 9-octadecenoic acid (Z) methyl ester differ significantly.
The ionization energy (I) or the minimum amount of energy required for removing the most loosely held electron, is comparatively low for more reactive and electron-donating molecules [22,8] . The low ionization energy of quercetin is justified by the fact that it acts as a more reactive inhibitor. The electron affinity (A) represents the energy that would be released upon gaining an electron [23]; in this paper, it is not compared with literature values, but a relatively high value of electron affinity is synonymous with the ability of a molecule to take up electrons from the metal surface.

The global softness (S) and hardness (η) provide another parameter to represent the interaction between the molecule and metal surface [24,25]; the soft molecules have low orbital energy difference and hence, act as more reactive in nature, just as the electron donation ability shows a soft molecule. A good inhibitor molecule will show a combination of high softness with low hardness. In this regard, quercetin stands out better than 9-Octadecenoic acid (Z) methyl ester again.

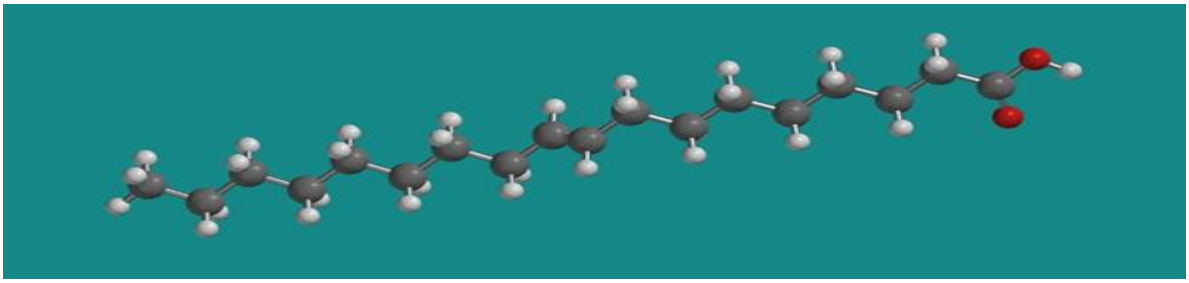

Fig 3: (a) Optimized Geometry of 9-Octadecenoic acid (Z) methyl ester Structure

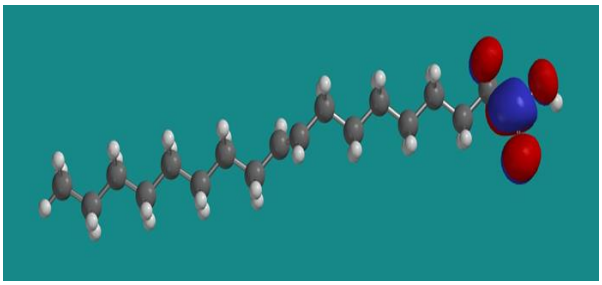

Fig 3: (b) E_{LUMO} (0.34 ev)

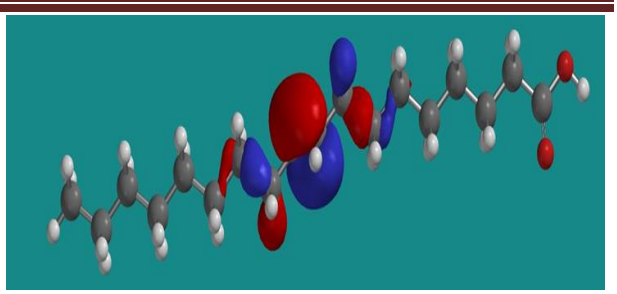

Fig 3: (c) E_{HOMO} (-6.38ev)

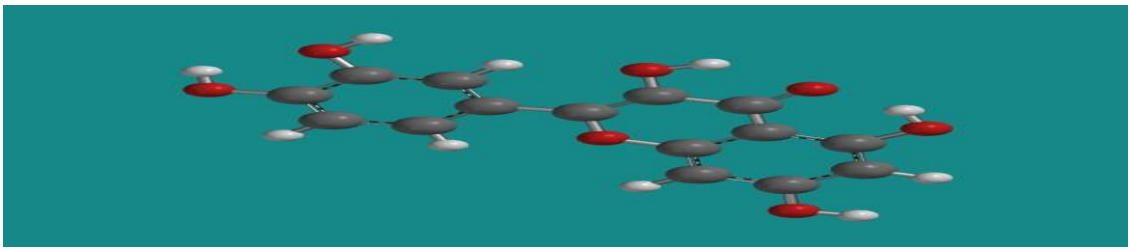

Fig 4: (a) Optimized Geometry of Quercetin

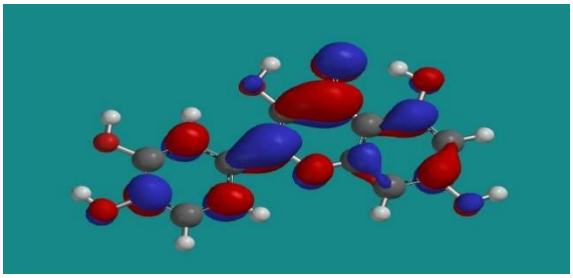

Fig 4: (b) E_{LUMO} (-1.84 ev)

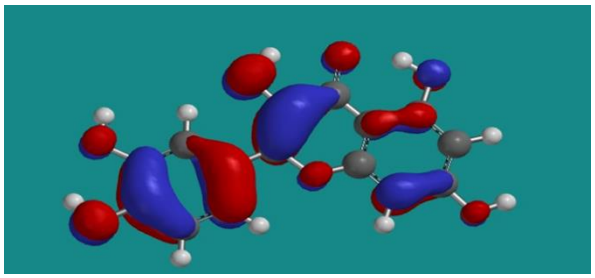

Fig 4 : (c) E_{HOMO} (-5.48ev)

Table 4: Quantum parameters for dye

S/N	Parameters	9 - octadecenoic acid	Quercetin
1	E_{HOMO} (ev)	-6.38	-5.48
2	E_{LUMO} (ev)	0.34	-1.84
3	Energy Gap (ΔE) (ev)	6.72	3.64
4	Ionisation potential (IP)	6.38	5.48
5	Electron Affinity (EA)	-0.34	1.84
6	Diapole Moment	1.35	0.27
7	Absolute Hardness (η)	3.36	1.82
8	Absolute Softness (σ)	0.30	0.55

CONCLUSION

The study shows that ethanolic extract of *Tectona grandis dye* is a good inhibitor of the corrosion of mild steel in acidic medium, the phytochemical analysis of the plant extracts shows that it contains some bio-molecule which aids in the inhibition efficiency. An increase in the concentration of extract increased corrosion inhibition efficiency on mild steel, but an increase in temperature decreased the efficiency of corrosion inhibition. 9-octadecenoic acid (Z) methyl ester and quercetin were some of the compounds identified in the extract through GC-MS and HPLC analyses, and through computational calculations, quercetin was predicted to be more efficient than 9-octadecenoic acid (Z). The agreement between the calculated and experimental results supports quantum chemistry as a useful approach for studying how organic molecules protect metals against corrosion.

Recommendations

Based on the findings, the theoretical and computational information obtained can be used in corrosion process optimization for the development of inhibitor which find applications in construction, oil and gas and metallurgical industry.

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