EFFICACY OF SEED EXTRACTS OF *MOMORDICA CHARANTIA* ON THE CORROSION INHIBITION OF MILD STEEL IN 1N HCl MEDIUM USING PHYTOCHEMICAL SCREENING, WEIGHT LOSS MEASUREMENTS AND QUANTUM CHEMICAL STUDIES

V. Kavitha[1], Dr. N. Gunavathy[2], S. Poovarasi[3]

[1] Doctorate scholar, Department of Chemistry, Nirmala College for Women, Coimbatore, Tamilnadu
[2] Assistant Professor, Department of Chemistry, Nirmala College for Women, Coimbatore, Tamilnadu
[3] PG student, Department of Chemistry, Nirmala College for Women, Coimbatore, Tamilnadu

ABSTRACT

Extract of Momordica Charantia Seed (MCS) was investigated as corrosion inhibitor of mild steel in 1N HCl using phytochemical screening, conventional weight loss, and theoretical analysis. Weight loss results showed that MCS seed extracts are good corrosion inhibitors. Inhibition efficiency increased with increase in concentration of inhibitor and decreased with temperature. The maximum inhibition efficiency was 95.06% in case of MCS extract in 1N HCl for immersion period of 7h at a concentration of 2.5 %v/v. Quantum studies revealed that inhibition was due to adsorption of active molecules leading to formation of a protective layer on surface of mild steel. Quantum chemical parameters such as highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) energy levels, HOMO–LUMO energy gap and electronic density were virtually identified. Quantum analysis demonstrated reactive centres of electrophilic and nucleophilic attack and strong inhibition properties of bioactive molecules of MCS extract.

Keyword: - *Momordica Charantia seed extract, phytochemical screening, weight loss, Quantum chemical parameters.*

1. INTRODUCTION

Mild steels are used extensively in chemicals as well as other allied industries. These structures are often subjected to cleaning, descaling and pickling by acids which are normally accompanied by considerable dissolution of metals as well as acid composition. Inhibitors are generally used to control metal dissolution. Non toxic inhibitor formulations are obtained from natural products which can replace those compounds that cause environment pollutants. Natural products are good source of eco friendly corrosion inhibitors. Extracts of naturally occurring plant products contain mixture of compounds and are biodegradable in nature and at the same time offer comparable performance and cost. Environmentally friendly corrosion inhibitors range from rare earth elements to organic compounds and are used as alternative corrosion inhibitors to reduce the harmful effects on humans, animals and environment.

From perspective of safety of metal against corrosion, non-toxic and effectiveness of inhibitors are considered more significant and desirable [1-7]. Quantum chemistry computations have been widely used to study reaction mechanisms and to interpret experimental results of compounds virtually [8]. Aim of this work was to investigate corrosion behaviour and mechanism for mild steel in solutions of 1N HCl with MCS extract by weight loss measurements and quantum studies.

2. MATERIALS AND METHODS

2.1 Collection of plant material and preparation of seed extracts

The study was carried out on M*omordica Charantia* seed (Fig-1). The sample was obtained from cultivated farm in Kalappatti, Coimbatore, India. Dried sample was ground into powder using an electronic blender, sieved and fine powder was stored in air tight container. 25 gm of dried powder of seed was boiled in 500ml of 1N HCl acid with reflux condenser for three hours and was kept overnight to extract its phytonutrients. The extract was filtered and

filtrate volume was made up to 500ml using the respective acids. The extract so prepared was taken as 5% stock solution and from this other concentrations were prepared (Fig-2).

Fig-1: MC Seed Powder

Fig-2: Photographs of Various Concentrations of the Plant Extract in Acid Medium

2.2 Phytochemical Screening on MCS

Screening of phytochemicals is significant for identification of bioactive principles present in plants. Phytochemical screening was carried out on MCS extracts by standard procedures [9]. Plant extracts were screened for reducing sugar, alkaloids, protein, phenols, flavonoids, amino acids, tannin, steroids, glycosides and saponins.

2.3 Materials Preparation

Corrosion tests were performed on coupons cut from sheets of mild steel of 2.0mm thickness obtained from Albert Steel House, Coimbatore, India. The chemical compositions of mild steel in terms of element weight percentage as given by supplier are shown in the Table 1.

Table-1: Chemical Composition of Mild Steel as Element Weight Percentage

S. No.	Name of the Element	Weight Percentage
1.	Carbon	0.123
2.	Manganese	0.031
3.	Silicon	0.011
4.	Phosphorus	0.037
5.	Sulphur	0.022
6.	Chromium	0.033
7.	Molybdenum	0.014
8.	Nickel	0.012
9.	Iron	Rest %

2.4 Weight loss measurements

Weight loss measurements were carried out using a SHIMADZU model AY 220. Mild steel specimens were immersed in beaker containing 100ml acid solution without and with different concentrations (0.10%v/v, 0.50%v/v, 1.00%v/v, 1.50%v/v, 2.00%v/v and 2.50%v/v) of MCS using glass hooks for a predetermined time period (1h, 3h, 5h, 7h, and 24h) at room temperature. For good reproducibility, experiment was carried out in triplicate. Test specimens were removed and washed with de-ionised water, dried and reweighed. From the weight loss, corrosion rate and inhibition efficiency were calculated.

Inhibition efficiency was calculated using formula [10],

$$IE\% = \frac{W_1 - W_2}{W_1} X\ 100 \quad (1)$$

Where, W_1 and W_2 are weight loss of mild steel after immersion in solutions without and with inhibitor respectively.

2.5 Quantum analysis

Computational analysis of molecular structures of MCS were done by MOPAC2016 [11] software using PM7 method. PM3 or Parameterized Model number 3, based on semi-empirical method for quantum calculation of molecular electronic structure in computational chemistry [12]. Positive and negative regions in HOMO and LUMO orbitals, Mulliken charges, Electrostatic potential map of compounds were computed using ArgusLab 4.0.1[13]. Structures of Vicine and Curcubitacin in MCS seed were obtained from literature for computational analysis.
3-Dimensional (3D) structures were retrieved from structural database and was optimized (Fig. 3) and taken as input file for quantum chemical studies.
Molecular properties like energy of highest occupied molecular orbital (E_{HOMO}), energy of lowest unoccupied molecular orbital (E_{LUMO}), global reactivity parameters such as chemical hardness (η), chemical potential (μ) and electrophilicity index (ω) were obtained to analyze reactivity of inhibitor molecules (Table 2). Electronegativity is measure of power of an electron or group of atoms to attract electrons towards it [14]. Molecular properties related to reactivity and selectivity of inhibitors like ionization potential (I), electron affinity (A), electronegativity (χ), global hardness (η) and softness (σ), were estimated according to Koopman's theorem [15] which relates to energy of HOMO and LUMO. Mulliken population analysis determines nucleophilic and electrophilic reaction centers in compounds.

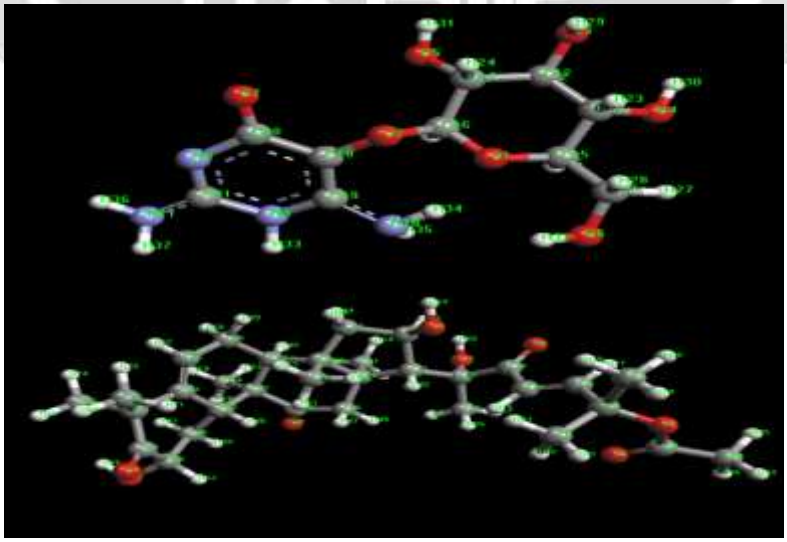

Fig-3: Molecular Structure of Vicine and Curcubitacin

Table-2: Quantum Chemical Parameters for Theoretical Analysis

S. No	Quantum parameters	formulation
1.	Chemical potential (μ)	$\mu = -\chi$
2.	Ionization potential (I)	$I = -E_{HOMO}$
3.	Electron affinity (A)	$A = -E_{LUMO}$
4.	Electronegativity (χ)	$\chi = \frac{I + A}{2}$
5.	Global hardness (η)	$\eta = \frac{I - A}{2}$
6.	Chemical softness (σ)	$\sigma = \frac{1}{\eta}$
7.	Electrophilicity index (ω	$\omega = \frac{\mu^2}{2\eta}$

3. RESULTS AND DISCUSSIONS

3.1 Phytochemical analysis

Plant analysis is devoted to the isolation and identification of secondary constituents in a particular species or group of species or species with expectation that some of constituents may be novel or of an unusual structure. Phytochemicals present in MCS in acid medium are summarized in Table-3.

Table-3: Phytochemical Constituents Present in Extract of MCS

Phytocompound	MCS	Phytocompound	MCS
Carbohydrates	–	Phlobatannins	–
Reducing sugar	++	Coumarins	–
Alkoloids	+	Cycloglycoside	–
Saponins	–	Total phenols	–
Tannins	++	Quinones	+
Flavonoids	++	Anthraquinones	++
Terpenoids	+	Steroids	++

Keywords: "++" active compound copiously present, "+" active compound present, "-" active compound absent

3.2 Weight loss Measurements

Mild steel was found to corrode in 1N HCl acid solution. This was proved by decrease in original weight of metal coupons. With addition of plant extract to acids, it was found that weight loss decreases with increase in concentration from 0.1 to 2.5% v/v due to adsorption of plant nutrient which protects the dissolution of metal.

Table-4 gives values of inhibition efficiency obtained from weight loss measurements of mild steel for various concentrations of MCS/1N HCl at 303K after different hours of immersion. The inhibition efficiency increased with increase in concentration of inhibitor from 0.1 to 2.5% at room temperature (Fig-4). Maximum inhibition efficiency was 95.06% in case of MCS /1N HCl for immersion period of 7h at a concentration of 2.5 %v/v (Fig- 4). These results suggest that adsorption model arrangement and orientation of constituents present in *Momordica Charantia* extract on surface of mild steel may change with time [16]. Decrease in inhibition efficiency thereafter with

increasing time may be due to shift in adsorption and desorption equilibria which takes place simultaneously on prolonged exposure to corrosive media [17]. Adsorbed organic molecules prevent further interaction of metal with acid. Protective film of a stable oxide of magnetite was formed on the mild steel. Magnetite adheres to the metal and results in an impermeable layer that stops further corrosion [18, 19].

Table-4: CR of Mild Steel and IE of MCS Extract in 1N HCl Acid in Various Concentration and Immersion Period

Conc. of extract (%)	1 h		3 h		5 h		7 h		24 h	
	CR mm/y	IE (%)	CR mm/y	IE (%)	CR mm/y	IE (%)	CR mm/y	IE (%)	CR mm/y	IE (%)
Blank	40.12	-	28.23	-	36.10	-	37.57	-	97.65	-
0.1	16.71	58.33	6.68	76.31	7.80	78.39	9.07	75.84	31.94	67.28
0.5	11.14	72.23	5.94	78.94	5.57	84.56	7.16	80.93	28.97	70.32
1.0	8.91	77.78	3.71	86.84	4.23	88.27	6.05	83.89	25.54	73.84
1.5	6.68	83.34	2.97	89.47	3.34	90.74	4.29	88.57	21.54	77.93
2.0	5.57	86.11	2.22	92.1	2.67	93.82	3.34	91.11	19.22	80.31
2.5	4.45	88.89	1.48	94.02	2.00	95.06	2.70	92.79	17.27	82.31

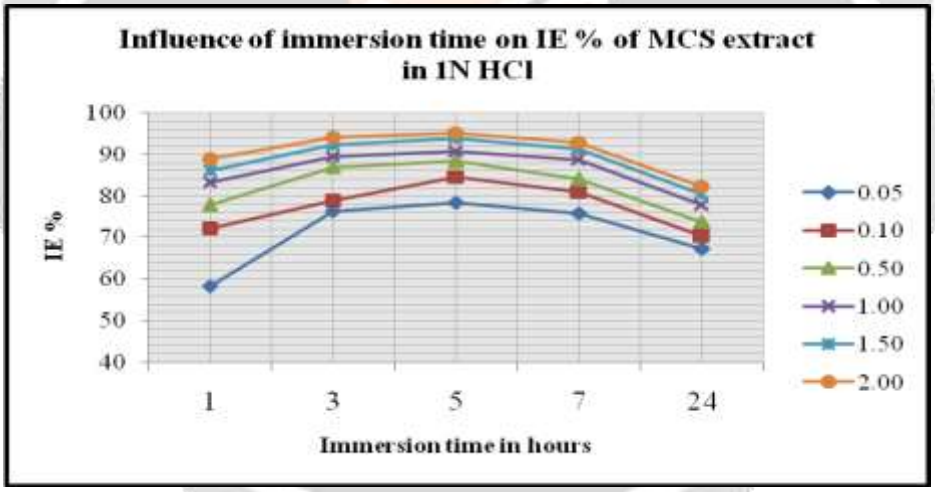

Fig-4: Influence of immersion time on IE % of MCS / 1N HCl

3.3 Quantum Chemical Parameters

Quantum chemical methods have been proved to be a very powerful tool for studying inhibition of corrosion of metals [20]. HOMO and LUMO density distribution for molecules were executed using MOPAC2016 with PM7 method. Positive and negative regions on HOMO and LUMO orbitals of molecules were computed using ArgusLab 4.0.1 (Fig. 5 and Fig. 6). The positive and negative phases of orbital are represented by two colours, blue regions represent an increase in electron density and red region represents a decrease in electron density [21].

E_{HOMO} measures electron donating ability of a compound to an appropriate acceptor molecule with low-energy empty molecular orbital. An inhibitor with higher HOMO energy can easily provide electrons for metallic substrate to adsorb on its surface [22-23]. Electrophilic attacks were shown to correlate with atomic sites having high density of the HOMO orbital, whereas nucleophilic attacks correlated well with atomic sites having high density of LUMO orbital (Kunichi Fukui was awarded the Nobel prize in chemistry in 1981 for developing this concept) [22,24].

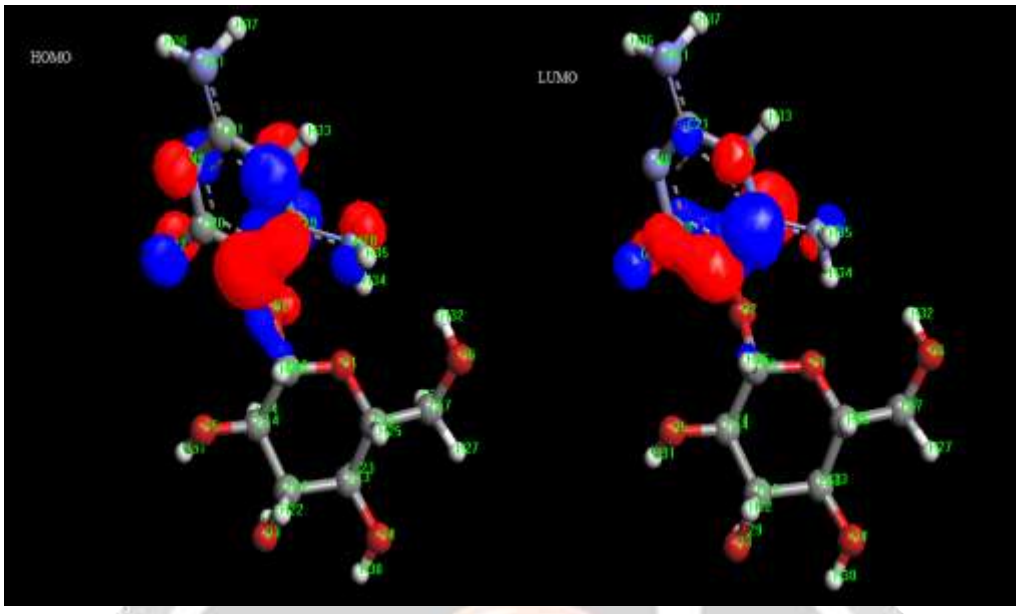

Fig-5: HOMO and LUMO Orbitals of Vicine

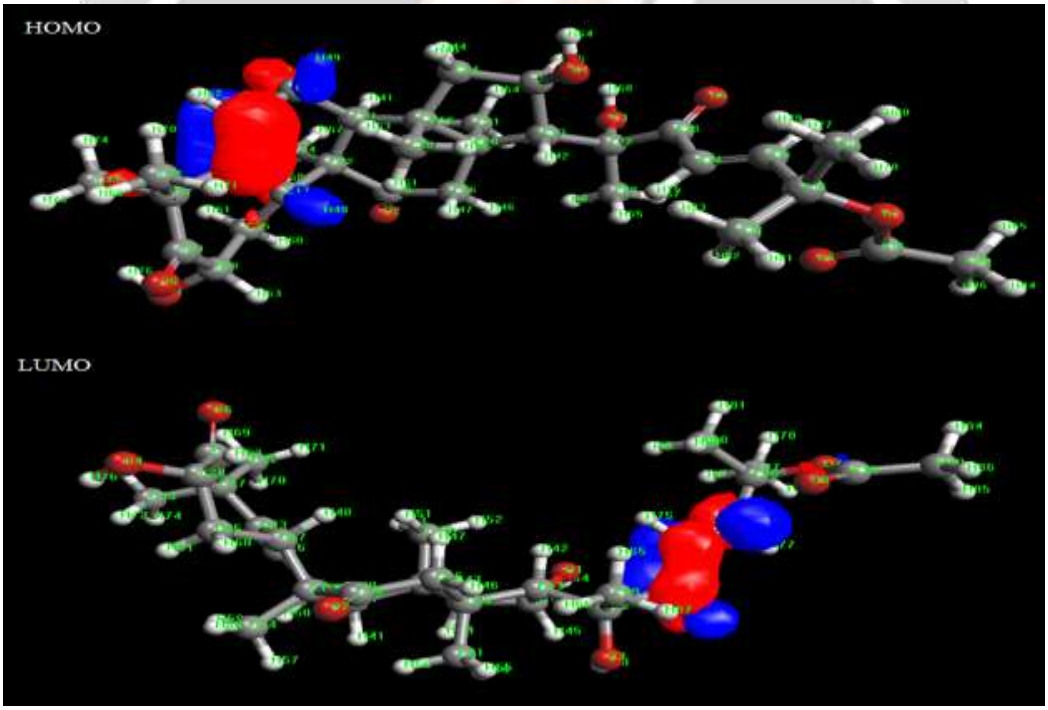

Fig-6: HOMO and LUMO orbitals of Curcubitacin

E_{LUMO} reveals tendency of a molecule to receive electrons. A molecule with lower LUMO energy would be a better electron acceptor from a donor molecule [25-27, 23]. It has been reported that inhibitor molecules can be adsorbed not only by donating electrons from their HOMO orbitals of Fe, but also by receiving electrons from metals to their LUMO molecular orbitals leading to create a feedback bond [25-27]. The molecule with highest E_{HOMO} value has highest tendency to donate electrons to appropriate acceptor molecule of low empty molecular orbital energy [28]. From results, it was evident that Curcubitacin had highest value of E_{HOMO} -8.490 (eV) and would be better adsorbed on metal surface and be a best corrosion inhibitor. As ΔE decreases, reactivity of molecule increases leading to increase in inhibition efficiency of molecule [29]. Low values of ΔE gap will render good inhibition efficiencies since energy to remove an electron from last occupied orbital will be minimized [30]. Quantum chemical parameters

obtained from theoretical calculations which are responsible for inhibition efficiency of compounds such as E_{HOMO}, $E_{LUMO,}$ energy gap (ΔE), dipole moment (μ), electronegativity (χ), electron affinity (EA), global hardness (η), softness (S), ionization energy (IE) and electrophilicity (ω) are shown in Table-5.

Table-5: Quantum Chemical Parameters of MCS Phytoconstituents

Parameters	**Vicine**	**Curcubitacin**
E_{HOMO} eV	-9.429	-8.491
E_{LUMO} eV	-0.458	-0.297
Energy Gap eV	8.971	8.193
IE	9.429	8.491
EA	0.458	0.297
χ	4.943	4.394
Ƞ	4.485	4.097
S	0.223	0.244
μ	-4.943	-4.394
ω	2.724	2.356

Energy gap (ΔE) values of the compounds show Curcubitacin < Vicine, which suggests that Curcubitacin had good reactivity and likely interact strongly with metal surface and act as good inhibitor. High ionization energy indicates high stability and chemical inertness and small ionization energy indicates high reactivity of atoms and molecules [31]. Low ionization energy 8.4905 (eV) of Curcubitacin indicates high inhibition efficiency. Absolute hardness and softness are important properties to measure molecular stability and reactivity.

A hard molecule has a large energy gap and a soft molecule has a small energy gap [32]. For simplest transfer of electron, adsorption could occur at part of molecule where softness (S), which is a local property, has a highest value [33]. Curcubitacin with softness value of 0.244 has highest inhibition efficiency. Curcubitacin with low hardness value 4.097 (eV) compared with other compounds have a low energy gap. Normally, inhibitor with least value of global hardness can be expected to have highest inhibition efficiency [34].

The Molecular Electrostatic Potential (MEP) measures the interaction of a positively charged point with nuclei and electrons of a molecule [35]. Quick Plot ESP (electrostatic potential) mapped density generated an electrostatic potential map on the total electron density contour of the molecule [36]. The interaction between the molecules is between regions of opposite electrostatic potential. Figure 7 and 8 shows the electrostatic potential map of Curcubitacin and Vicine in which areas of colour, shade "in blue" suggest potential of positive values, i.e electron deficiency; while the shades of colour areas "red" indicates negative values of the electrostatic potential, that is, regions rich in electrons [37].

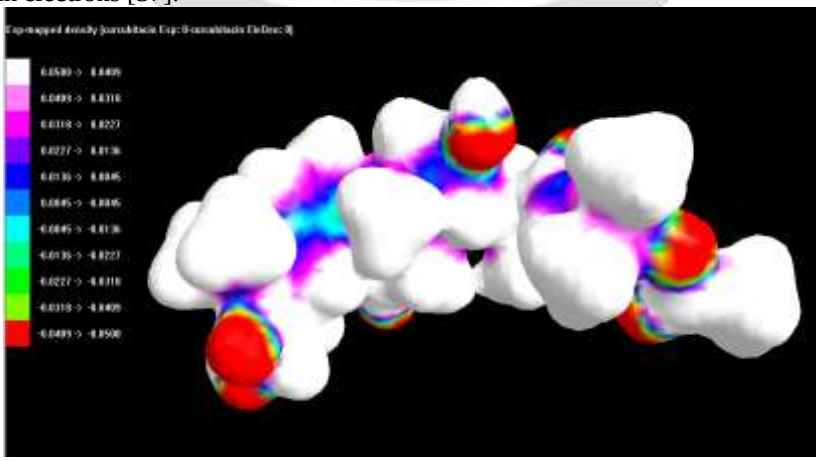

Fig-7: ESP Mapped Density of Curcubitacin

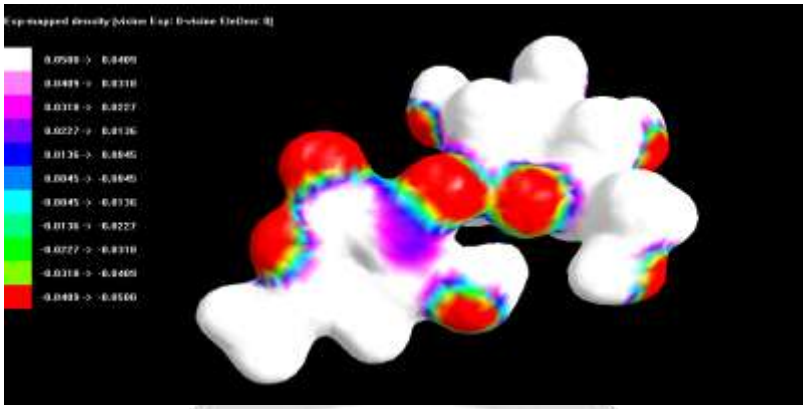

Fig-8: ESP Mapped Density of Vicine

3.4 Mulliken Charge Distributions on Compounds

Mulliken population analysis is mostly used for calculation of charge distribution in a molecule [38]. Mulliken charge distribution of Vicine and Curcubitacin are presented in Table 6 and 7. More negative atomic charges of adsorbed centre, more easily atom donates its electron to unoccupied orbital of metal [39]. Mulliken charges of compounds show that there was more than one active centre in molecules. More negative atomic charges of adsorbed centre, more easily atom donates its electron to unoccupied orbital of metal [40].

Table-6: Mulliken Charge Distribution on Vicine

Vicine		Vicine		Vicine		Vicine	
Atoms	**Charge**	**Atoms**	**Charge**	**Atoms**	**Charge**	**Atoms**	**Charge**
O1	-0.2938	**N10**	-0.0548	**C19**	-0.1452	**H28**	0.1033
O2	-0.1520	**N11**	-0.0095	**C20**	0.3983	**H29**	0.2133
O3	-0.3139	**C12**	-0.1009	**C21**	-0.0462	**H30**	0.2348
O4	-0.3169	**C13**	-0.0545	**H22**	0.1778	**H31**	0.2317
O5	-0.2966	**C14**	-0.0626	**H23**	0.1229	**H32**	0.2175
O6	-0.3180	**C15**	-0.0500	**H24**	0.1403	**H33**	0.1384
O7	-0.3080	**C16**	0.1281	**H25**	0.1457	**H34**	0.1364
N8	0.0801	**C17**	-0.0848	**H26**	0.1386	**H35**	0.0857
N9	-0.2766	**C18**	-0.1502	**H27**	0.1494	**H36**	0.1181
						H37	0.0742

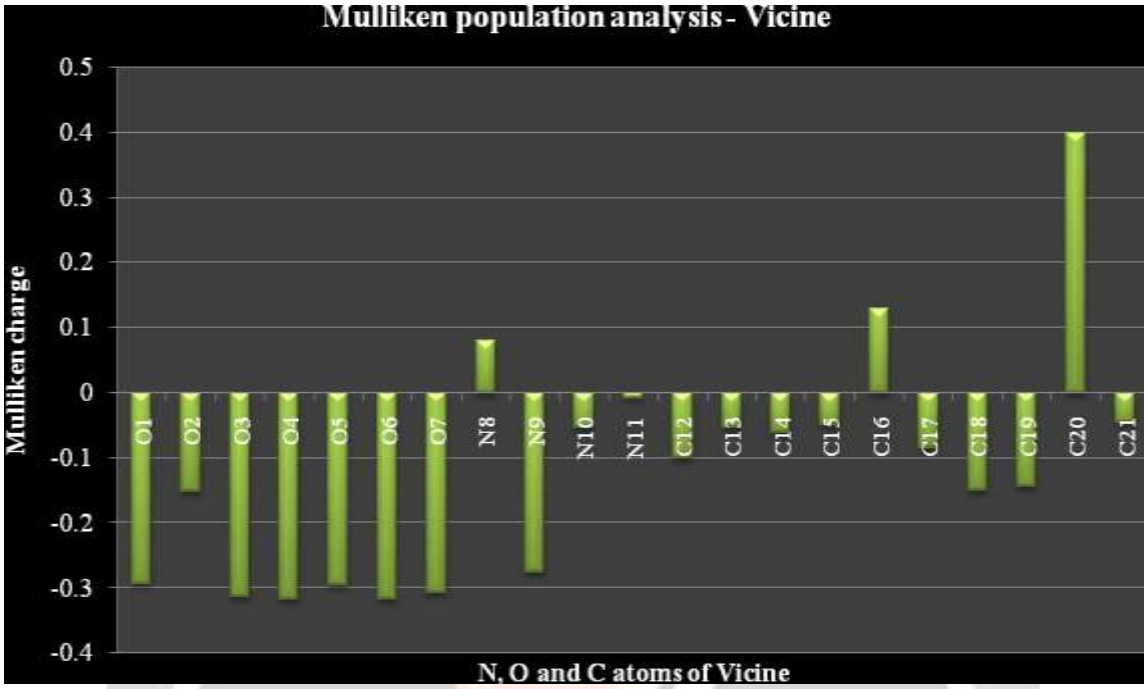

Fig-9: Mulliken charge distribution of N, O and C atoms of Vicine molecule.

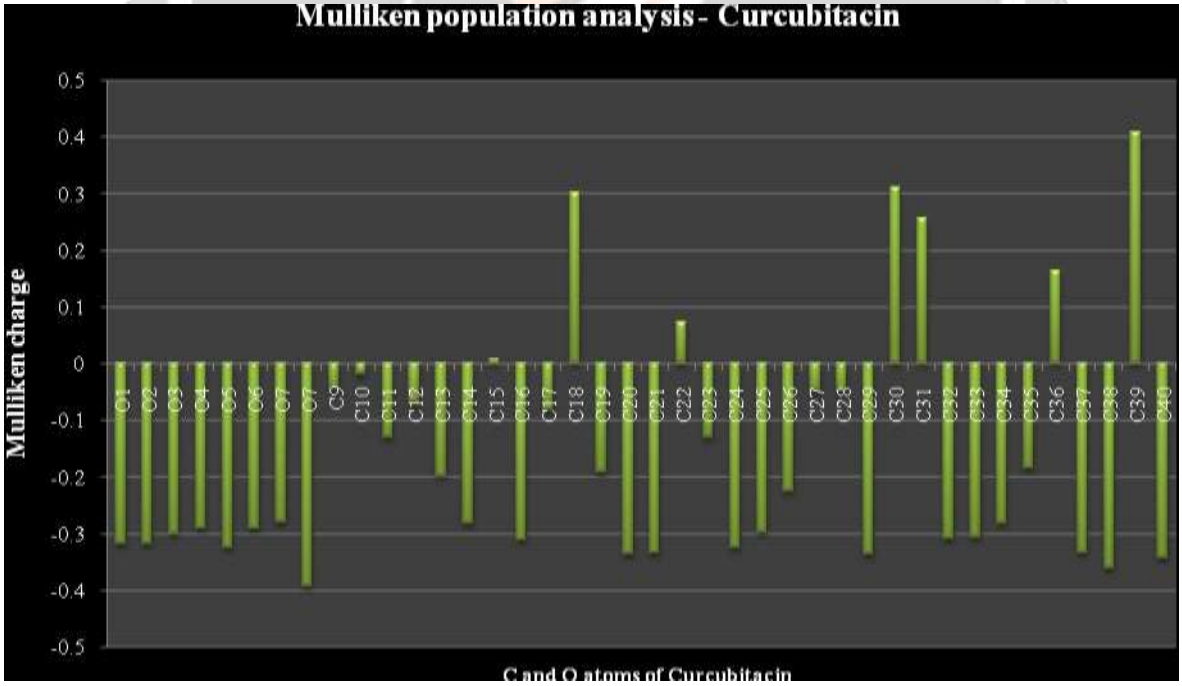

Fig-10: Mulliken Charge Distribution on C and O Atoms of Curcubitacin Molecule

Table-7: Mulliken Charge Distribution on Curcubitacin

Curcubitacin		Curcubitacin		Curcubitacin		Curcubitacin		Curcubitacin	
Atoms	**Charge**	**Atoms**	**Charge**	**Atoms**	**Charge**	**Atoms**	**Charge**	**Atoms**	**Charge**
O1	-0.3192	**C20**	-0.3370	**C39**	0.4087	**H58**	0.1381	**H77**	0.2131
O2	-0.3195	**C21**	-0.3350	**C40**	-0.3441	**H59**	0.1181	**H78**	0.1225
O3	-0.3009	**C22**	0.0722	**H41**	0.1449	**H60**	0.1702	**H79**	0.1230
O4	-0.2912	**C23**	-0.1304	**H42**	0.1680	**H61**	0.1364	**H80**	0.1223
O5	-0.3266	**C24**	-0.3260	**H43**	0.1388	**H62**	0.1939	**H81**	0.1246
O6	-0.2919	**C25**	-0.2975	**H44**	0.1317	**H63**	0.1651	**H82**	0.1428
O7	-0.2811	**C26**	-0.2270	**H45**	0.1033	**H64**	0.2213	**H83**	0.1217
O7	-0.3936	**C27**	-0.0499	**H46**	0.1698	**H65**	0.1221	**H84**	0.1404
C9	-0.0446	**C28**	-0.0492	**H47**	0.1506	**H66**	0.1249	**H85**	0.1411
C10	-0.0207	**C29**	-0.3369	**H48**	0.1463	**H67**	0.1399		
C11	-0.1315	**C30**	0.3097	**H49**	0.1337	**H68**	0.2251		
C12	-0.0697	**C31**	0.2551	**H50**	0.1318	**H69**	0.1321		
C13	-0.1998	**C32**	-0.3089	**H51**	0.1100	**H70**	0.1069		
C14	-0.2816	**C33**	-0.3074	**H52**	0.1292	**H71**	0.1206		
C15	0.0080	**C34**	-0.2827	**H53**	0.1316	**H72**	0.1046		
C16	-0.3122	**C35**	-0.1856	**H54**	0.1119	**H73**	0.1237		
C17	-0.0825	**C36**	0.1634	**H55**	0.1493	**H74**	0.1191		
C18	0.3004	**C37**	-0.3349	**H56**	0.1135	**H75**	**0.**2094		
C19	-0.1922	**C38**	-0.3610	**H57**	0.1129	**H76**	0.2098		

It could be readily observed that oxygen and some carbon atoms have high charge densities. Mulliken charge is a measurement of local reactivity as well as indicative of local nucleophilic or electrophilic feature in molecules [41]. Figure 9 and 10 shows Mulliken charge distribution of all heteroatoms and some of carbon atoms are negatively charged. Thus, considered as active sites for adsorption process of inhibitor molecule onto the mild steel surface [42]. Curcubitacin has more electronegative O8 and O5 with charges -0.3936 and -0.3266. In Curcubitacin, C40, C20, C29, C21, C37, O8 and O5 are most susceptible sites for electrophilic attacks as they present highest values of negative charge. On other hand, C39, C30 and C18 in Curcubitacin are most susceptible sites for the nucleophilic attacks as they present highest values of positive charge. The regions of highest electron density are generally sites to which electrophiles can attack [43]. Vicine has more electronegative O6, O3 and O4 with charges -0.3180, -0.3139 and -0.3169 that shows due to more electron-donating nature of atoms and region for electrophilic attack. The susceptible sites for nucleophilic attacks possess highest values of positive charge at C20. O and C atoms were active centers that possess strong ability of bonding to metal surface. Therefore, Curcubitacin and Vicine can accept electrons from metal through these atoms and hence these compounds could serve as good corrosion inhibitor against metal surface protection.

4. CONCLUSION

Based on the above results, following conclusion can be drawn,

- Phytochemical screening, weight loss measurements, and quantum analysis confirmed the corrosion preventive property of MCS in 1N HCl medium. The investigation shows MCS extract as an excellent inhibitor for mild steel corrosion in 1N HCl.
- The qualitative analysis of MCS showed the presence of alkaloids, saponins, tannins, flavonoids, terpenoids, coumarins, phenols and steroids.

- Weight loss measurements establish that inhibition efficiency increased with increase in concentration of inhibitor from 0.1% v/v to 2.5% v/v at room temperature. MCS extract had 95.06% inhibition efficiency in 1N HCl for the immersion period of 7h at 2.5 %v/v
- From quantum analysis on bioactive molecules of MCS, Curcubitacin had highest inhibition efficiency because it possessed highest E_{HOMO} energy in comparison with the other derivatives and it was more capable of offering electrons.
- Mulliken population analysis on Vicine and Curcubitacin possess sites for nucleophilic and electrophilic attacks that aid adsorption on to mild steel surface as obtained from quantum chemical calculations. The Quantum chemical calculations are also in good agreement with the experimental results.

All the result of investigation indicates that MCS in acid can be used as corrosion inhibitors for mild steel. Further, as these extracts are environmental friendly, they can be considered as green corrosion inhibitors.

5. REFERENCES

1. E. Chaieb, A. Boulanger, B. Hammouti, M. Berrabah, Limonene as green inhibitor for steel corrosion in Hydrochloric Acid, Acta Physico-Chimica Sinica , Vol 25, pp. 1254, 2009.
2. E. El Ouariachi, J. Paolini, M. Bouklah, A. Elidrissi, A. Bouyanzer, B. Hammouti, J.-M. Desjobert, J. Costa, Adsorption properties of Rosmarinus officinalis oil as green corrosion inhibitors on C38 steel in 0.5 M H_2SO_4, Acta Metallurgica Sinica (English letters), Vol. 23, No.1, pp. 13-20, 2010.
3. Z. Faska, A. Bellioua, M. Bouklah, L. Majidi, R. Fihi, A. Bouyanzer, B. Hammouti, Effect of pulegone and pulegone oxide on the corrosion of steel in 1 M HCl, Monatshefte für Chemie, Vol. 139, pp. 1417, 2008.
4. Chris O. Akalezi, Conrad K. Enenebaku, Emeka E. Oguzie, Inhibition of acid corrosion of mild steel by biomass extract from the petersianthus macrocarpus plant, Journal of Materials and Environmental Science, Vol. 4, No. 2, pp. 217-226, 2013.
5. M. Ramananda Singh, A green Approach:A corrosion inhibition of mild steel by adhatoda vasica plant extract in 0.5 M H_2SO_4, Journal of Materials and Environmental Science , Vol. 4, No. 1, 2013, pp. 117-126.
6. O. Benali, H. Benmehdi, O. Hasnaoui, C. Selles, R. Salghi, Green corrosion inhibitor: inhibitive action of tannin extract of Chamaerops humilis plant for the corrosion of mild steel in 0.5 M H_2SO_4, Journal of Materials and Environmental Science, Vol. 4, No. 1, pp. 127-138, 2013.
7. R. Saratha, V. G. Vasudha, Inhibition of Mild Steel Corrosion in 1N H_2SO_4 Medium by Acid Extract of Nyctanthes arbortristis Leaves, E-J. Chem, Vol. 6, pp. 1003-1008, 2009.
8. V. Kavitha, N. Gunavathy, Computational Investigations on Curcumin and Demethoxycurcumin as Corrosion Inhibitors: A Comparative Analysis. International Journal of Science & Engineering Development Research, Vol.2, No. 3, pp.18 - 24, 2017.
9. J. B. Harborne. Phytochemical methods: A guide to modern technique of plant analysis, Champman and Hall, 1998.
10. O. Lahodny-Sarc, F.Kapor, Corrosion inhibition of carbon steel in the near neutral media by blends of tannin and calcium gluconate, Mater. Corros., Vol. 53, No. 4, 264–268. 11, 2002.
11. J. J. P. Stewart, Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters, J. Mol. Model., Vol. 19, no. 1, pp. 1–32, 2013.
12. J. J. P. Stewart, Optimization of parameters for semiempirical methods I. Method, J. Comput. Chem., vol. 10, no. 2, pp. 209, 1989.
13. M. A. Thompson, Molecular docking using ArgusLab, an efficient shape-based search algorithm and AScore scoring function, in Proc. ACS Meeting, Philadelphia, Pa, USA, p. 172, 2004.
14. L. Pauling, The Nature of the Chemical Bond, Coruell University Press, Ithaca, New York, 1960.
15. T. Koopmans, Uber die Zuordnung von Wellenfunktionen und Eigenwerten zu den einzelnen Elektronen eines Atoms,Physica, Vol. 1, pp.104–113, 1933.
16. N. Rekha, Shashi Sharma, I. K. Sharma, P. S. Verma, Alka Sharma, Inhibitor efficacy of Piper Nigrum Linn. Extract on corrosion of AA1100 in HCl Rasayan J Chem, Vol. 3, pp. 783-795, 2010.
17. V. Kavitha, Dr. N. Gunavathy, Mild Steel Corrosion Inhibition by Daucus carota Pulp Extract in 1N Hydrochloric Acid Medium, International Journal of Scientific Research in Science and Technology, Vol 2, No 6 , pp.249-256, 2016.
18. O. Lahodny-Sarc, F.Kapor, Corrosion inhibition of carbon steel in the near neutral media by blends of tannin and calcium gluconate, Mater. Corros., Nol. 53, No. 4, 264–268. 11, 2002.

19. E. Almeida, D. Pereira, M. O. Figueiredo, V. M. M. Lobo, M. Morcillo, The influence of the interfacial conditions on rust conversion by phosphoric acid. Corros. Sci., Vol. 39, no. 9, pp. 1561–1570, 1997.
20. K. F. Khaled, K. Babic-Samardzija N. Hackerman, Theoretical study of the structural effects of polymethylene amines on corrosion inhibition of iron in acid solutions, Electrochim. Acta, Vol. 50, pp. 2515-2520, 2005.
21. K. Laxmi, Theoretical Approach on structural aspects of antiepileptic agent indoline-2,3-dione-3-oxime by arguslab 4 software, J. Appl. Chem., Vol. 2, No.1, pp. 92-101, 2014.
22. K. Laxmi, A Hypothetical Study on Structural aspects of Indole - 3 - carbinol (I3C) by Hyperchem and Arguslab 4 software, Int. Journal of Engineering Research and Applications, Vol. 6, No. 1, pp.17-24, 2016
23. A.Y. Musa, W. Ahmoda, A.A. Al-Amiery, A.A.H. Kadhum, A.B. Mohamad, Quantum chemical calculation for the inhibitory effect of compounds, *J.* Struct. Chem., Vol. 54, No. 2, pp. 301-308, 2013.
24. Swayansiddha Tripathy, Susanta Kumar Sahu, Structural aspects and Docking studies of 3-{5-[4-oxo-2-thioxo-3-(3-trifluoromethylphenyl)-thiazolidin-5-ylidenemethyl] furan-2-yl}-benzoic acid (OTBA) an antibacterial drug targets FtsZ protein, Int. J. Pharma. Sci., Vol. 6, No. 3, pp. 1534-1539, 2016.
25. N. Soltani, N. Tavakkoli, M. Khayatkashani, M. R. Jalali, A. Mosavizade, Green Approach to Corrosion Inhibition of 304 Stainless Steel in Hydrochloric Acid Solution by the Extract of Saliva officinalis leaves, Corros. Sci., Vol. 62, pp. 122-135, 2012.
26. Z. El Adnani, M. Mcharfi, M. Sfaira, M. Benzakour, A.T. Benjelloun and M. EbnTouhami, DFT theoretical study of 7-R-3methylquinoxalin-2(1H)-thiones (Rdouble bond; length as m-dashH; CH3; Cl) as corrosion inhibitors in hydrochloric acid, Corros. Sci., Vol. 68, pp.223–230, 2013.
27. M.S. Morad and A.M. Kamal El-Dean, 2, 2′-Dithiobis (3-cyano-4,6-dimethylpyridine): A new class of acid corrosion inhibitors for mild steel, Corros. Sci., Vol. 48, No. 11, pp. 3398–3412., 2006.
28. G. Gece, S. Bilgic, Quantum chemical study of some cyclic nitrogen compounds as corrosion inhibitors of steel in NaCl media, Corros. Sci., Vol. 51, No. 8, pp. 1876-1878, 2009.
29. M.K. Awad, M.S. Mustafa, M.M. Abo Elnga, Computational simulation of the molecular structure of some triazoles as inhibitors for the corrosion of metal surface, J. Mol. Struct.. (Theochem), Vol. 959, No. 1, pp. 66-74, 2010.
30. C. O. Akalezi, C. K. Enenebaku, E. E. Oguzie, Application of aqueous extracts of coffee senna for control of mild steel corrosion in acidic environments, Int. J. Indus. Chem., Vol. 3, pp. 13-25, 2012.
31. T. Chakraborty, K. Gazi , D. C. Ghosh, Computation of the atomic radii through the conjoint action of the effective nuclear charge and the ionization energy, Mol. Phys., Vol. 108, no. 16, pp. 2081-2092, 2010.
32. N. O. Obi-Egbedi, I. B. Obot, M. I. El-Khaiary, S. A. Umoren, E. E. Ebenso, Computational Simulation and Statistical Analysis on the Relationship between Corrosion Inhibition Efficiency and Molecular Structure of Some Phenanthroline Derivatives on Mild Steel Surface, Int. J. Electrochem. Sci., Vol. 6, pp. 5649-5675, 2011.
33. R. Hasanov, M. Sadikoğlu, S. Bilgiç, Electrochemical and quantum chemical studies of some Schiff bases on the corrosion of steel in H_2SO_4 solution, Appl. Surf. Sci., Vol. 253, pp. 3913-3921, 2007.
34. E. E. Ebenso, D. A. Isabirye and N. O. Eddy, Adsorption and Quantum Chemical Studies on the Inhibition Potentials of Some Thiosemicarbazides for the Corrosion of Mild Steel in Acidic Medium, Int. J. Mol. Sci., Vol. 11, No. 6, pp. 2473-2498, 2010.
35. Williams, D. E.; Comprehensive Chemical Kinetics. Rev. Comp. Chem., Vol 2, pp. 226, 1991.
36. Laxmi K.Theoretical Approach on structural aspects of antiepileptic agent indoline-2,3-dione-3-oxime by arguslab 4 software. Journal of Applied Chemistry, Vol 2, No 1, pp. 92-101, 2014.
37. G.A.Araujo, E.P.Silva, R.G.Sanabio, J.A.Pinheiro, M.B. Albuquerque, R.R.Castro, M.M. Marinho, F.K.S.Lima, E.S.Marinho. Characterization in Silico of the Structural Parameters of the Antifungal Agent Ketoconazole .Biological and Chemical Research, Vol. 3, pp. 133-142 | Science Signpost Publishing
38. J. N. Murrell, S.F. Kettle, J.M. Tedder, The Chemical Bond, John Wiley & Sons, Chichester, 1985.
39. S. Xia, M. Qiu, L. Yu, F. Liu, H. Zhao, Molecular dynamics and density functional theory study on relationship between structure of imidazoline derivatives and inhibition performance, Corros. Sci., Vol. 50, No. 7, pp. 2021–2029, 2008.
40. J. Fu , S. Li, Y. Wang , J. Mater. Sci, Vol 45, 6255, 2010.
41. L. Larabi, O. Benali, S. M. Mekelleche, Y. Harek. Appl. Surf. Sci, Vol 253, No. 3, pp. 1371 – 1378, 2006
42. R Lgaz, M. Salghi, M. Larouj, S. Elfaydy, H.Jodeh , Abbout, Lakhrissi,K. Toumiat, H. Oudda. Corrosion inhibition of mild steel in hydrochloric acid by 5,5',5''-(nitrilotris (methylene)) tris-(8-quinolinol): Experimental, theoretical and molecular dynamic studies. Moroccan Journal of Chemistry, Vol. 4, No. 2, pp.592-612, 2016.

43. A.Y. Musa, A. H. Kadhum, A. B. Mohamad, A. B. Rahoma and H. Mesmari, Electrochemical and quantum chemical calculations on 4, 4-dimethyloxazolidine-2-thione as inhibitor for mild steel corrosion in hydrochloric acid, J. Mol. Struct., Vol. 969, No. 1, pp. 233-237, 2010.

BIOGRAPHIES

	V. Kavitha is Doctorate scholar at the Department of Chemistry, Nirmala College for Women, Coimbatore, Tamilnadu. She is pursuing her Ph.D degree in chemistry under guidance of Dr.N.Gunavathy in field of Corrosion science. Her research is related to electrochemistry, green corrosion inhibitor and quantum chemical studies.
	Dr. N. Gunavathy is Assistant Professor at the Department of Chemistry, Nirmala College for Women, Coimbatore, Tamilnadu. She received her Ph.D. degree in Chemistry from Anna University. She received All India level University Gold medal from, The President of India, Dr.A.P.J.ABDUL KALAM for standing first in the examination for Bachelor of Education (B.Ed) in December 2003, IGNOU, New Delhi. She is member of Member of Indian Science Congress Association. Dr. N. Gunavathy has more than 29 publications in the fields of electrochemistry, corrosion science, inorganic chemistry and cheminformatics. She has been regularly reviewing scientific and technical articles for international journals.
	S. Poovarasi is student at the Department of Chemistry, Nirmala College for Women, Coimbatore, Tamilnadu. She received her M. Sc in Chemistry from Bharathiar University. She is dynamic in her research work in corrosion inhibitors.