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Theoretical evaluation of corrosion inhibitor potential of *Phoenix Dactylifera L.* extracts

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ABSTRACT

Phoenix Dactylifera L. is a dioeceous plant belonging to the Arcacaea family which means it has separate male and female saplings. The present study involves identification of phytochemicals of male and female date palm hexane extracts by Gas chromatography mass spectrometry followed by quantum mechanical analysis. Different quantum mechanical parameters like ionization potential, electron affinity, energy gap, global hardness, global softness, electronegativity and electron back donation are evaluated for each phytoconstituent. The optimum condition for a particular phytochemical as potent corrosion inhibitor is higher value of HOMO, global softness, back donation and lower values of LUMO, electrophilicity, global hardness and ionization potential. The study concludes that corrosion inhibition potential of male date palm extract is attributed to synergistic action of the compounds phytol, n-hexadecanoic acid, 9,12,15-Octadecatrienoic acid and Squalene. The corrosion inhibition potential of female date extracts is due to synergistic action of , n-hexadecanoic acid, 9,12,15-Octadecatrienoic and oleic acid.

KEYWORDS: Phoenix Dactylifera L., corrosion, Squalene, phytol, phytochemicals

1. INTRODUCTION

Corrosion can be defined as retrogression of metal on its chemical or electrochemical interaction with surroundings [1]. As an aftermath of this natural and spontaneous process pure metals and/or metal alloys are converted into their various stable forms such as sulfides, oxides, hydroxides and so on [2]. The approximate global annual cost of corrosion is USD 2.5 trillion which is 3-4 % of the global gross domestic product [3]. Corrosion processes are conveyed by numerous reactions which results in change of composition of both metal surface and local surroundings i.e. formation of oxides, local pH variations, electrochemical potential and migration of metal ions into the coating matrix [4]. The degradation of metal upon its interaction with surroundings can be classified into two classes: Dry corrosion and Wet corrosion. Dry corrosion arises upon interaction of metals with gases at elevated temperatures. Wet corrosion takes place due to interaction of metals with aqueous solutions or electrolytes [5]. Corrosion inhibitors are chemical compounds which assuage corrosion progression when added in minor amounts to the corrosive domain [6]. Derivatives of phosphates & chromates, synthetic organic compounds, nanomaterials, plant extracts and polymeric substances have been used to prevent corrosion. However, the utilization of plants extracts enriched with tannins, alkaloids, flavanoids, tannins, amino acids, anthraquinones and saponins as corrosion inhibitors is beneficial due to their cost-effective, eco-friendly, plentiful availability and simplified production techniques [7-14].

Emad E. El Katori et al. evaluated the corrosion inhibition of aluminum by *Bassia muricata* extract in 1 M H_2SO_4 acidic medium at different concentrations in temperature range 298-313 K. The maximum inhibitor efficiency was found to be 90% at inhibitor concentration 300 ppm. The adsorption behavior of *B. muricata* extract on the surface of aluminum is best fitted to Temkin adsorption isotherm model [15]. Kumar et. al. evaluated *Asparagus Racemosus* as a corrosion inhibitor of aluminum under 1 M HCl acidic conditions. The maximum inhibitor efficiency was found to be 74.4% at inhibitor concentration 6000 ppm, The adsorption behavior of *Asparagus Racemosus* on the surface of aluminum well fitted to Langmuir adsorption isotherm [16]. The adsorption of Areca Palm leaf extract on the surface of aluminum in 0.5M HCl acidic medium was best described by Langmuir adsorption isotherm. Charge transfer process restricts dissolution of Al in HCl medium [17]. The adsorption of *Jasminum nudiflorum Lindl.* leaves extract on the surface of aluminum under 1N HCl acidic conditions is in accordance with Langmuir adsorption isotherm. The maximum inhibitor efficiency for inhibitor concentration 1 g L^{-1} was found to be 93.1% at 20^0C temperature for immersion time 2 hours. Different methods used to evaluated corrosion inhibitor potential include mass loss measurements, polarization studies, electronic impedance measurements and gasometric analysis [18].

Phoenix Dactylifera L. also known as date palm is monocotyledonous plant belonging to arecaceae family [19]. Date palm is dioeceous that means it has separate male and female saplings [20]. In the present study, hexane extracts of male and female *Phoenix Dactylifera L.* leaves are analyzed by Gas chromatography mass spectrometry so as to identify phytochemicals comprised. These phytochemicals were then subjected to quantum mechanical analysis to evaluated their corrosion inhibitor potential.

2. EXPERIMENTAL WORK

Preparation of male and female *Phoenix Dactylifera L.* extracts:

Male and female *Phoenix Dactylifera L.* leaves were collected in the month of December from Anjar city of Kachchh region. They were washed with distilled water, dried under shade, powdered and further adapted in the experiment. For the preparation of extracts, 10 gm of male and female *Phoenix Dactylifera L.* leaves were macerated with 100 ml hexane for 24 hours with occasional stirring. The resultant extract was filtered and utilized for the experiment.

GC-MS analysis of male and female *Phoenix Dactylifera L.* extracts:

GC-MS analysis was carried using Shimadzu GC-MS QP 2010 using helium as carrier gas . Name, molecular weight and molecular structure of each detected compounds was accomplished by comparing mass spectra of unknown compound with mass spectra of standard compound found in database of NIST 11 , NIST 11s and Wiley library.

Quantum mechanical analysis of phytoconstituents of Male & Female *Phoenix Dactylifera L.* extracts:

E_{HOMO}, E_{LUMO} values of identified constituents by GC-MS were obtained using pit quantum repository portal [21].

3. RESULTS & DISCUSSION

Quantum mechanical parameters of phytoconstituents of ethyl acetate extracts of male and female *Phoenix Dactylifera L.* leaves were calculated using the following equation [22]:

$$E = E_{HOMO} - E_{LUMO} \text{ ----1}$$

$$A = -E_{LUMO} \text{ ----2}$$

$$I = -E_{HOMO} \text{ -----3}$$

$$X = \frac{I+A}{2} \text{ ----4}$$

$$\eta = \frac{I-A}{2} \text{ ----5}$$

$$\sigma = \frac{1}{\eta} \text{ ----6}$$

$$\omega = \frac{X^2}{2\eta} \text{ -----7}$$

$$E_{(back\ donation} = \frac{-\eta}{4} \text{ ----8}$$

Here E= band gap (eV) , E_{HOMO} and E_{LUMO} are the energies of HOMO and LUMO (eV) respectively, A =

electron affinity, I = ionization potential, X= electronegativity, η = global hardness, σ = global softness, ω = electrophilicity and $E_{(back\ donation)}$ = back donation potential [22].

Table 1: Retention time, relative percentage and name of phytoconstituents identified using NIST and WILEY library from Gas Chromatogram in male date palm leaves hexane extract

Sr. no	Retention time (min)	Relative percentage	Compound name
A1	12.69	1.83	tetradecane
A2	15.16	2.00	Hexadecane
A3	17.37	3.03	nonadecane
A4	17.76	5.09	Phytol
A5	18.19	1.45	neophytadiene
A6	18.89	34.39	n-hexadecanoic acid
A7	19.39	1.77	octadecane
A8	20.49	9.86	9,12,15-Octadecatrienoic acid
A9	20.76	2.07	Octadecanoic acid
A10	26.16	3.19	Squalene
A11	28.10	0.55	Dodecane

Table 2: Retention time, relative percentage and name of phytoconstituents identified using NIST and WILEY library from Gas Chromatogram in female date palm leaves hexane extract

Sr. no	Retention time	Relative percentage	Compound name
B1	9.91	1.14	Dodecane
B2	12.69	1.65	tetradecane
B3	15.16	0.55	eicosane
B4.	17.03	2.62	6,10,14-Trimethyl-2-pentadecanone
B5	17.67	4.12	neophytadiene
B6	18.88	22.15	n-hexadecanoic acid
B7	20.36	8.05	Phytol
B8	20.45	8.19	Oxacycloheptadec-8-en-2-one
B9	20.48	6.69	9,12,15-Octadecatrienoic acid
B10	20.52	5.13	Oleic Acid
B11	24.74	4.25	Methyl commate b
B12	26.11	10.53	Lupeol

Table 3: Quantum mechanical parameters of phytochemicals of male *Phoenix Dactylifera L.* extract

Sr.no	E HOMO (eV)	E LUMO(eV)	(A)	(I)	χ
A1	-10.77	6.8	-6.8	10.77	1.99
A2	-10.73	6.79	-6.79	10.73	1.97
A3	-10.69	6.78	-6.78	10.69	1.96
A4	-9.32	1.22	-1.22	9.32	4.05
A5	-9.85	3.82	-3.82	9.85	3.02
A6	-8.95	-0.68	0.68	8.95	4.82
A7	-10.71	6.79	-6.79	10.71	1.96
A8	-9.5	0.94	-0.94	9.5	4.28
A9	-10.81	3.98	-3.98	10.81	3.42
A10	-8.85	1.28	-1.28	8.85	3.79
A11	-10.82	6.82	-6.82	10.82	2.00

Table 3(Continue): Quantum mechanical parameters of phytochemicals of male *Phoenix Dactylifera L.* extract

Sr.no	(E)	(n)	(σ	(w)	E(back donation)
A1	17.57	8.79	0.11	0.22	2.20
A2	17.52	8.76	0.11	0.22	2.19
A3	17.47	8.74	0.11	0.22	2.18
A4	10.54	5.27	0.19	1.56	1.32
A5	13.67	6.84	0.15	0.66	1.71
A6	8.27	4.14	0.24	2.80	1.03
A7	17.50	8.75	0.11	0.22	2.19
A8	10.44	5.22	0.19	1.75	1.31
A9	14.79	7.40	0.14	0.79	1.85
A10	10.13	5.07	0.20	1.41	1.27
A11	17.64	8.82	0.11	0.23	2.21

Table 4: Quantum mechanical parameters of phytochemicals of female *Phoenix Dactylifera L.* extract

Sr.no	E HOMO (eV)	E LUMO(eV)	(A)	(I)	χ
B1	-10.82	6.82	-6.82	10.82	2.00
B2	-10.77	6.8	-6.80	10.77	1.99
B3	-8.02	-0.31	0.31	8.02	4.17
B4	-10.08	0.96	-0.96	10.08	4.56
B5	-9.85	3.82	-3.82	9.85	3.02
B6	-8.95	-0.68	0.68	8.95	4.82
B7	-9.32	1.22	-1.22	9.32	4.05
B8	-9.53	1.29	-1.29	9.53	4.12
B9	-9.5	0.94	-0.94	9.50	4.28
B10	-9.62	0.9	-0.90	9.62	4.36
B11	-8.99	4.33	-4.33	8.99	2.33

Table 4(Continue): Quantum mechanical parameters of phytochemicals of female *Phoenix Dactylifera L.* extract

Sr.no	(E)	(n)	(σ	(w)	E(back donation)
B1	17.64	8.82	0.11	0.23	2.21
B2	17.57	8.79	0.11	0.22	2.20
B3	7.71	3.86	0.26	2.25	0.96
B4	11.04	5.52	0.18	1.88	1.38
B5	13.67	6.84	0.15	0.66	1.71
B6	8.27	4.14	0.24	2.80	1.03
B7	10.54	5.27	0.19	1.56	1.32
B8	10.82	5.41	0.18	1.57	1.35
B9	10.44	5.22	0.19	1.75	1.31
B10	10.52	5.26	0.19	1.81	1.32
B11	13.32	6.66	0.15	0.41	1.67

From the above table 1, we see that male *Phoenix Dactylifera L.* extract is comprised of tetradecane, hexadecane, nonadecane, phytol, neophytadiene, n-hexadecanoic acid, octadecane, 9,12,15-Octadecatrienoic acid, Octadecanoic acid, Squalene and dodecane. It is evident from table 2 that female *Phoenix Dactylifera L.* extract consists of dodecane, tetradecane, eicosane, neophytadiene, n-hexadecanoic acid, 6,10,14-Trimethyl-2-pentadecanone, phytol, 9,12,15-Octadecatrienoic acid, Oxacycloheptadec-8-en-2-one, oleic acid , lupeol and methyl commate B. The given study involves evaluation of different quantum mechanical parameters such as band gap E (eV) , E_{HOMO} and E_{LUMO} are the energies of HOMO and LUMO (eV) respectively, electron affinity A, ionization potential I, electronegativity X, global hardness η, global softness σ, electrophilicity ω and back donation potential $E_{(back\ donation)}$. The energy level of HOMO orbital signifies tendency of donating an electron to low lying metal orbital. So, higher energy of HOMO orbital increases the ability of a inhibitor molecule to give away electrons and higher the inhibitor potential of the molecule. For male *Phoenix Dactylifera L.* , the energy level of HOMO can be shown as A10>A6>A4>A8>A5>A3>A7>A2>A1>A9>A11.

Similarly, for the female date palm extract energy level of HOMO can be shown as B3>B6>B11>B7>B9>B8>B12>B10>B5>B4>B2>B1. The energy level of LUMO indicates the tendency of a molecule to accept the electrons. Hence lesser the energy value of LUMO, higher is the inhibitor efficiency of a molecule to avert the corrosion of metal. Compounds with lowest value of band gap are enhanced corrosion inhibitors. For male *Phoenix Dactylifera L.* extract, the order of band gap can be shown as A6<A10<A8<A4<A5<A9<A3<A7<A2<A1<A11. The order of band gap for female *Phoenix Dactylifera L.* extract is represented as B3<B6<B9<B10<B7<B12<B8<B4<B11<B5<B2<B1. The constituents with low global hardness (n) and high global softness (σ) exhibits enhanced potential to donate electrons to the metal surface and hence form the protective layer on the metal surface and thereby reducing corrosion. Considering the compounds A6,A10,A8 and A4 for male *Phoenix Dactylifera L.* extract , the trend of global hardness can be written as A6<A10<A8<A4. For the female extract, considering the compounds B3,B6,B9 and B10, the order of global hardness can be shown as B3<B6<B9<B10. The trend of global softness is reverse of that of global hardness. Anti-corrosive property of compound is improved with decrease in electronegativity. The ionization potential I and electron affinity A indicates electron donating and electron accepting tendency of the molecules. More the value of ionization potential lower is electron donating tendency of a inhibitor molecule. Higher the value of electron affinity, higher is the tendency of a molecule to accept electrons. Compounds A10 and B3 of male and female date palm respectively shows the least ionization potential. Electrophilicity ω signifies for the stabilization of inhibitor molecules on the surface of metal. Lower the values of electrophilicity more is the electron donating potential and stabilization of the inhibitor molecules on the surface of metals. Considering the compounds A6,A10, A8 and A4 for male *Phoenix Dactylifera L.* extract , the trend of electrophilicity can be shown as A10<A4<A8<A6. For the female extract, considering the compounds B3,B6,B9 and B10, the order of electrophilicity can be shown as B9<B10<B3<B6. Back donation is the tendency of a molecule to accept electrons from d-orbital of metal. Corrosion inhibition properties of a molecule increases

with increase in back donation. Among the compounds, A10, A4, A6 and A8 of male extract, compound A4 possess highest back donation. Similarly among the compounds B3,B6,B9 and B10 of female extracts , B10 possess highest back donation property [22-24].

4. CONCLUSION

In the present study , theoretical evaluation of phytoconstituents of male and female date palm leaves hexane extracts is carried to evaluate their potential to inhibit corrosion. The study concludes that a compound with enhanced corrosion inhibition property is that which exhibits higher value of HOMO, global softness, back donation and lower values of LUMO, electrophilicity, global hardness and ionization potential. The corrosion inhibition potential of male date palm extract could be attributed to the synergistic action of phytol, n-hexadecanoic acid, 9,12,15-Octadecatrienoic acid and Squalene. The corrosion inhibition tendency of female date palm extract is due synergistic action of eicosane, n-hexadecanoic acid, 9,12,15-Octadecatrienoic and oleic acid.

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Conflict of interest statement

Authors declare that they do not have any conflict of interest.

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