

Full Paper

Theoretical Studies of Anti-corrosion Properties of Triphenylimidazole Derivatives in Corrosion Inhibition of Carbon Steel in Acidic Media via DFT Approach

Oyebamiji Abel Kolawole and Semire Banjo

Department of Pure and Applied Chemistry, Faculty of Pure and Applied Sciences, Ladoko Akintola, University of Technology, P.M.B. 4000, Ogbomosh, Oyo State, Nigeria

*Corresponding Author, Tel.: +2348038269809

E-Mail: bsemire@lautech.edu.ng

Received: 21 August 2017 / Received in revised form: 9 November 2017 /

Accepted: 23 November 2017 / Published online: 31 January 2018

Abstract- Quantum chemical calculations via B3LYP/6-31G(d,p) level were carried out on 2,4,5-triphenyl-4,5-dihydro-1H-imidazole (**P1**) and 2-(4,5-diphenyl-4,5-dihydro-1H-imidazol-2-yl)phenol (**P2**) which were used as corrosion inhibitors for carbon steel in acidic media. The parameters like HOMO and LUMO energies, energy band gap, dipole moment, chemical potential (μ), chemical hardness (η) and global nucleophilicity (ω) were calculated and argued in relation to the observed inhibitory efficiency for the studied compounds. Also, the effect of hydroxyl group substituent on the operation of corrosion inhibition of Triphenylimidazole derivatives was observed.

Keywords- Triphenylimidazole derivatives, Corrosion Inhibition, Molecular Descriptors, Carbon Steel, DFT

1. INTRODUCTION

The use of mild steel in several industries as one of the major ingredients in the production of pipes for construction works has gained a global attention. It was considered to be very imperative in any construction projects like conduits, bridges, construction of buildings and weighty automobiles [1-4]. The widely preferred use of mild steel by

researchers and in industries is a function of its fairly low cost and high mechanical strength [5]. Conversely, mild steel get rusted effortlessly in wet and acidic environments which were activated by acid wash, engraving and/or prickling of metal surface [6].

Several literatures have revealed many important activities of imidazole derivatives such as anti-corrosion activity [7], antimicrobial activity [8-16], anti-inflammatory [17-21] etc. Also, imidazole and its derivatives as essential class of heterocyclic compounds displays a wide range of activities which made many scientists over the years to uphold their desire in the use of sulphur and nitrogen-containing heterocyclic compounds [22]. More so, Debus *et al.*, in 1858 first reported the synthesis of imidazole from diketone, an aldehyde and ammonia; nevertheless, in 1840, several imidazole derivatives through other means had been discovered and reported as well [23,24].

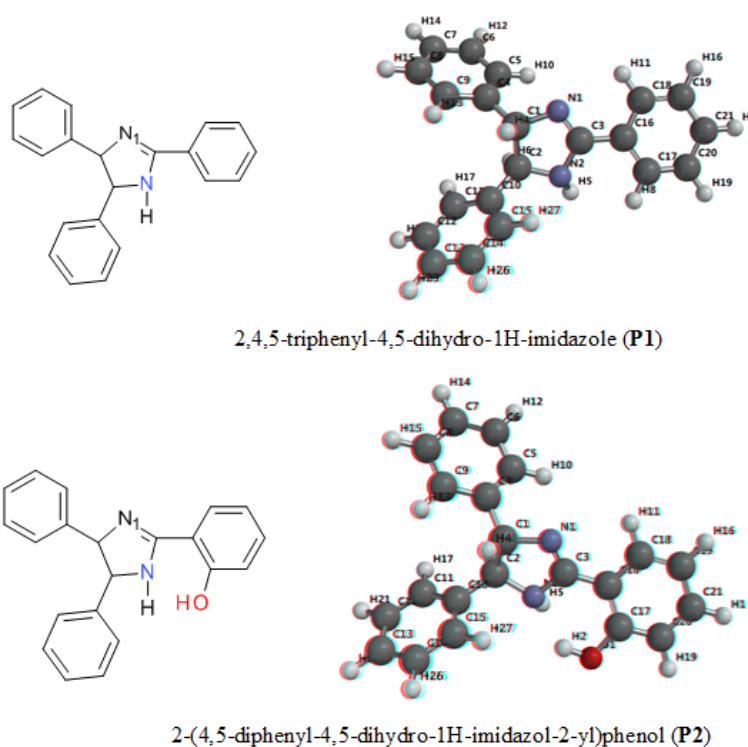


Fig. 1. Schematic and optimized structures with labeling of the studied compounds [7]

Moreover, the use of quantum chemical calculation in the study of corrosion inhibition has now gained a global attention amidst scientists [25]. This had been attributed to the highly significant role it played in explicating the electronic structure and reactivity of compounds [26]. Although, there were other methods used in computational chemistry, but density functional theory (DFT) has turned to a very efficient technique in building new measures for justifying, predicting and understanding chemical processes [27]. Nowadays, quantum chemical calculation via density functional theory helps to identify the corrosion inhibitory descriptors by relating the experimental facts to calculated molecular descriptors

like HOMO energy, LUMO energy, band gap energy, dipole moment, charges on every heteroatoms etc. [28-32].

Therefore, the major aim of this paper is to use quantum chemical calculations via density functional theory (DFT) method to probe the corrosion inhibiting competence of derivatives of Triphenylimidazole compounds against the corrosion of carbon steel as it has been experimentally established by Mouhsine *et al.*, 2017 [7] to be efficient as corrosion inhibiting agents. Thus, two molecular compounds (2,4,5-triphenyl-4,5-dihydro-1H-imidazole [**P1**] and 2-(4,5-diphenyl-4,5-dihydro-1H-imidazol-2-yl)phenol) [**P2**]) were observed in this research work as displayed in Figure 1.

2. COMPUTATIONAL DETAILS

The studied compounds were subjected to theoretical calculation with the use of density functional theory with B3LYP functional via 6-31G** basis set. The calculated molecules were first optimized in gas phase and then optimized in water. Over the years, density functional theory has gained a greater popularity and this can be attributed to its efficient approximation of molecular descriptors linked to molecular reactivity [33]. Therefore, DFT calculations offer theoretical evidence for qualitative chemical observation such as chemical hardness (η), electronegativity (χ), global electrophilicity index (ω), local reactivity index, softness (s), electron affinity and ionization potential are all defined in terms of the HOMO and the LUMO energies which was related to Koopmans' theorem [34] and the estimation were carried out using equation: **Chemical potential** and electronegativity are related as:

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

Chemical hardness (η): this defines the resistance of a molecule to a charge transfer and this can be calculated using the equation:

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

Global electrophilicity (ω): this defines the electrophilic propensity of a molecule and it can be calculated using the equation:

$$\omega = \frac{\mu^2}{2\eta} \quad (3)$$

Number of electrons transfer (ΔN) can be calculated using:

$$\Delta N = \frac{\chi_{Fe} - \chi_{inh}}{2(\eta_{Fe} + \eta_{inh})} \quad [35, 36] \quad (4)$$

Where χ_{Fe} and χ_{inh} means the absolute electronegativity of metal (Fe) and the inhibitor molecule respectively as well as η_{Fe} and η_{inh} signify absolute hardness of metal (Fe) and the

inhibitor molecule respectively. Also, the chosen values for χ_{Fe} and η_{Fe} are 7 eVmol⁻¹ and 0 eVmol⁻¹ respectively [37].

Moreover, the Local reactivity index explains the reactivity of definite molecular atom in connection to the adhesion of an organic inhibitor to a precise metallic surface.

Also, the disparity in electron density for a nucleophile $f^+_{(r)}$ and $f^-_{(r)}$ as the Funki functions can be calculated by the determinate variances calculation [38];

$$f^+_{(r)} = q_{kN+1(r)} - q_{kN(r)} \quad (\text{for nucleophilic attack}) \quad (5)$$

$$f^-_{(r)} = q_{kN(r)} - q_{kN-1(r)} \quad (\text{for electrophilic attack}) \quad (6)$$

Where $q_{kN+1(r)}$, $q_{kN(r)}$ as well as $q_{kN-1(r)}$ are the electronic densities of anionic, neutral and cationic species respectively.

3. RESULTS AND DISCUSSION

3.1. Molecular descriptors

As reported in this work, several pertinent quantum chemical descriptors obtained from the studied molecules which include the HOMO energy, the LUMO energy, the band gap, dipole moment, the chemical hardness (η), chemical potential, global nucleophilicity, area, volume, log P, molecular weight, Ovality, electron transfer, polar surface area, heteroatom, polarization, HBA and HBD were listed in Table 1 and 2.

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

	HOMO	LUMO	BG	DM (Debye)	CH	CP	GN	AREA	VOL
P1	-6.05	-0.97	5.08	3.04	2.54	-3.51	2.43	344.52	330.92
P2	-6.03	-0.95	5.08	2.69	2.54	-3.49	2.40	350.52	337.43

Table 2. Selected molecular descriptors obtained by B3LYP/6-31G** (Continuation)

LOGP	MW	OVALITY	ΔN	PSA	HET	POL	HBA	HBD	%IE
2.72	298.389	1.49	0.68	18.71	-1.145	67.02	1	0	92.3
1.64	314.388	1.50	0.69	34.38	-1.737	67.54	2	1	97.1

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are very noteworthy descriptors for the prediction of the effectiveness of a chemical varieties. HOMO is usually known to be linked with the capability of a molecular compound to donate electron to the neighboring molecules. Also, increasing HOMO energy

brings about increasing inhibition efficiency [39]. Therefore, the calculated HOMO energies for compound **P1** and **P2** were -6.05eV and -6.03eV respectively. As shown in Table 1, **P2** with highest HOMO energy proved to have highest inhibition efficiency. So, as reported by Chandrabhan *et al.*, 2016, the inhibitor molecules with electron donating group, displays reasonably higher inhibition efficiency. Thus, the adsorption of inhibiting molecule on the surface of the metal could be expedited through the existence of apposite functional groups [40,41]. Therefore, in Table 2, inhibition efficiencies could be ordered as **P2>P1**; this could be accredited to higher electron donating tendency of $-\text{OH}$ group, that also improved its knack to bequeath charges to the surface of the metal during the adsorption process [42]. Figure 2 showed the HOMO and LUMO orbitals overlay for the studied compounds.

More so, lowest unoccupied molecular orbital energy with lower value revealed that the studied molecular compound has the ability to receive electrons from the neighboring compound that has the ability to donate [43]. The calculated LUMO energy value was -0.97eV for **P1** and -0.95eV for **P2**; this showed that **P1** with lowest LUMO value will be readily available to receive electron from d-orbital of disintegrating steel. The band gap energy ($E_{\text{LUMO}} - E_{\text{HOMO}}$) presented facts about the general reactivity of molecular compounds. Also as reported by Eddy, 2010, the lower the band gap energy, the better the reactivity of a molecular compounds [44]. Therefore, as shown in Table 1, **P1** and **P2** have the same band gap energy.

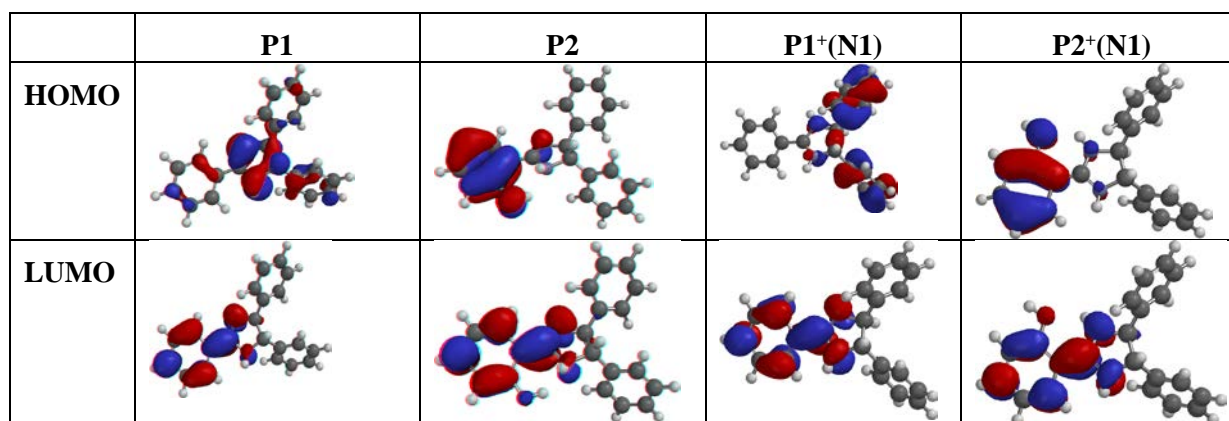


Fig. 2. The HOMO and LUMO orbitals overlay for the studied compounds

Furthermore, another vital electronic descriptor (Dipole moment), which was observed to be resulted from non-uniformed sharing of electronic charges on several atoms in the molecular compound [45] showed no correlation with the observed inhibition efficiency, since the molecule with high inhibitor and high dipole moment will be suitable to form strong dipole–dipole interactions with the surface of iron, which will then lead to firm adsorption on the iron surface [46]. Also, estimation of the centres of adsorption of inhibitors could be achieved via apposite descriptors such as mulliken population analysis which was used in the

calculation of charge distribution density over the molecule. The charge density on N1 and N2 were $-0.550e$ and $-0.595e$ respectively for **P1** and for **P2**, N1(-0.529), N2(-0.623) and O1(-0.585). More so, according to Breke *et al.*, 2002, it was reported that the more negatively charged a heteroatom is, the more tendency for it to be adsorbed on the metallic surface [47]; so, imidazole in this studied compound is most likely site for adsorption. In addition, as shown in Table 1 and 2, Chemical potential, area, volume, molecular weight, ovality, PSA, polarizability, HBA and HBD increased as the %IE increased while global nucleophilicity and log P showed an inverse correlation with the observed %IE (i.e. decreasing with increasing % IE).

In addition, the amount of electrons transmitted (ΔN) described the tendency of a molecular compound to bequeath electrons; and as it was reported by Gomez *et al.*, 2006 that the higher the amount of electrons transmitted, the higher the tendency of a compound to give electrons to the neighboring molecular compound that lack electron [48]. Thus, higher predilection of an anti-corrosive molecule to relate with the surface of the metal is a function of a higher amount of electrons transmitted (ΔN) [49]. Also, according to Lukovits *et al.*, 2001, if $\Delta N < 3.6$, the molecular compounds may be presumed to retain charge transfer capacity towards the surface of the metal [50]. Therefore, the ΔN values obtained for the studied inhibitors showed their inclination to bequeath electrons to the metal surface.

3.2. Molecular properties of protonated P1 and P2

In this research, **P1** and **P2** were protonated in aqueous medium at B3LYP/6-31G** level. The protonation site which brought about lower molecular energy were found on N1 for both molecules as shown in Figure 1, though, there was opportunity of adding another proton at N2 in both **P1** and **P2**, nevertheless lowermost energy molecular structures acquired were put into consideration (Table 3). The bond length (N1-C1, C2-N2 and C3-N1) calculated for $P1^+(N1)$ were 1.474\AA , 1.474\AA and 1.328\AA compared to 1.470\AA , 1.471\AA and 1.288\AA for **P1**. This revealed that N1-C1, C2-N2 and C3-N1 for $P1^+(N1)$ were elongated and this made it to experience bond localization.

Table 3. Energies and Selected Geometries of the Neutral and Protonated Species

Inhibitor	HOMO (eV)	LUMO (eV)	ΔE (eV)	Energy (au)	N1-C1 (Å)	C1-C2 (Å)	C2-N2 (Å)	N2-C3 (Å)	C3-N1 (Å)
P1	-6.05	-0.97	5.08	-920.621276	1.470	1.581	1.471	1.398	1.288
$P1^+(N1)$	-6.55	-1.60	4.95	-921.098881	1.474	1.574	1.474	1.328	1.328
P2	-6.03	-0.95	5.08	-995.846450	1.467	1.581	1.481	1.420	1.283
$P2^+(N1)$	-6.48	-1.66	4.82	-996.326180	1.472	1.571	1.470	1.327	1.337

$P1^+(N1)$ and $P2^+(N1)$: Protonated Molecule **P1** and **P2**

Nevertheless, in protonation, C1-C2 and N2-C3 for P1⁺(N1) were shortened when compared to neutral (P1). Also, for P2⁺(N1), the calculated N1-C1 and C3-N1 bond lengths were 1.472Å and 1.337Å respectively. More so, it was noted that these were elongated in comparison to neutral inhibitor (P2).

According to Semire *et al.*, 2013, it was observed that the role played by calculated dihedral angle which shows the planarity of molecules cannot be toiled with in adsorption of inhibitor on the surface of metals [51]. In this study, it was observed that both neutral and protonated corrosion inhibitors tend towards planarity, although the neutral species tends toward planarity at C₁₆C₃N₁C₁ than the protonated, while it was slightly distorted than protonated species at C₁₆C₃N₂C₂. The calculated dihedral angle for P1, P1⁺(N1), P2 and P2⁺(N1) were -178.14° (C₁₆C₃N₁C₁), -167.45°(C₁₆C₃N₂C₂), 175.74° (C₁₆C₃N₁C₁), -175.74°(C₁₆C₃N₂C₂), -176.63° (C₁₆C₃N₁C₁), -172.17°(C₁₆C₃N₂C₂), -175.72° (C₁₆C₃N₁C₁), -174.72°(C₁₆C₃N₂C₂) respectively. More so, the energy for the studied molecules were calculated and reported as shown in Table 3.

Table 4. Fukui Indices for Nucleophilic and Electrophilic Attacks for Inhibitor P1

ATOM	P _{N+1(r)}	P _{N-1(r)}	P _{N(r)}	f_k^+	f_k^-
C1	0.008	-0.025	0.003	0.005	0.028
C2	-0.003	-0.009	0.000	-0.003	0.009
C3	0.438	0.516	0.441	-0.003	-0.075
C4	0.081	0.142	0.11	-0.029	-0.032
C5	-0.165	-0.098	-0.13	-0.035	-0.032
C6	-0.066	-0.115	-0.088	0.022	0.027
C7	-0.081	-0.085	-0.09	0.009	-0.005
C8	-0.071	-0.117	-0.093	0.022	0.024
C9	-0.106	-0.101	-0.118	0.012	-0.017
C10	0.097	0.153	0.124	-0.027	-0.029
C11	-0.113	-0.099	-0.121	0.008	-0.022
C12	-0.075	-0.115	-0.097	0.022	0.018
C13	-0.082	-0.074	-0.091	0.009	-0.017
C14	-0.070	-0.116	-0.093	0.023	0.023
C15	-0.148	-0.086	-0.120	-0.028	-0.034
C16	0.013	0.108	0.065	-0.052	-0.043
C17	-0.177	-0.086	-0.107	-0.070	-0.021
C18	-0.194	-0.093	-0.115	-0.079	-0.022
C19	-0.095	-0.106	-0.083	-0.012	0.023
C20	-0.108	-0.114	-0.094	-0.014	0.020
C21	-0.172	-0.063	-0.077	-0.095	-0.014
N1	-0.685	-0.385	-0.550	-0.135	-0.165
N2	-0.654	-0.494	-0.595	-0.059	-0.101

Moreover, Figure 2 showed frontier molecular orbital (HOMO, HOMO-1, LUMO and LUMO+1) for P1, P1⁺ (N1), P2 and P2⁺ (N1) respectively. The study of electronic features of protonated compounds exposed modifications in chemical properties, for example, ability of the inhibitors to donate electron to the metal. Thus, the calculated HOMO of the protonated compounds (P1⁺(N1) and P2⁺(N1)) is lower than the neutral molecules (P1 and P2), and this revealed that protonation reduced the ability of P1⁺(N1) and P2⁺(N1) to donate electron.

Table 5. Fukui Indices for Nucleophilic and Electrophilic Attacks for Inhibitor P2

ATOM	$P_{N+1(r)}$	$P_{N-1(r)}$	$P_{N(r)}$	f_k^+	f_k^-
C1	0.004	0.006	0.000	0.004	-0.006
C2	-0.022	-0.004	-0.014	-0.008	-0.010
C3	0.389	0.375	0.414	-0.025	0.039
C4	0.076	0.119	0.103	-0.027	-0.016
C5	-0.172	-0.099	-0.135	-0.037	-0.036
C6	-0.066	-0.111	-0.089	0.023	0.022
C7	-0.08	-0.097	-0.089	0.009	0.008
C8	-0.072	-0.113	-0.093	0.021	0.020
C9	-0.103	-0.125	-0.114	0.011	0.011
C10	0.125	0.158	0.146	-0.021	-0.012
C11	-0.118	-0.136	-0.125	0.007	0.011
C12	-0.075	-0.116	-0.096	0.021	0.020
C13	-0.081	-0.098	-0.09	0.009	0.008
C14	-0.072	-0.118	-0.093	0.021	0.025
C15	-0.152	-0.093	-0.125	-0.027	-0.032
C16	0.003	0.137	0.071	-0.068	-0.066
C17	0.288	0.328	0.281	0.007	-0.047
C18	-0.224	-0.069	-0.126	-0.098	-0.057
C19	-0.094	0.013	-0.095	0.001	-0.108
C20	-0.158	-0.011	-0.104	-0.054	-0.093
C21	-0.166	-0.045	-0.077	-0.089	-0.032
N1	-0.663	-0.443	-0.529	-0.134	-0.086
N2	-0.662	-0.61	-0.623	-0.039	-0.013
O1	-0.630	-0.435	-0.585	-0.045	-0.150

However, protonated molecules have lower LUMO energy than the neutral molecule and this showed that protonation increased the ability of the inhibitors to accept electron from the d-orbital of the metal [52]. More so, lower band gaps together with structural steadiness should support the adsorption of protonated molecules on the surface of metal. Thus, it is proposed that there will be adsorption of more protonated molecules on the surface of metal at low concentrations. Nevertheless, desorption of the protonated would be swift from metal surface due to charge repulsion at high concentrations and molecular distortion of the

molecules from planarity; this accelerates the adsorption of non-protonated molecules on the surface of metal at equilibrium [51].

3.3. Local Reactivity Descriptors

Fukui functions apprise the centers where nucleophilic (f_k^+), electrophilic (f_k^-) and radical reactions have the highest probability to occur in a molecular compound. Equation 5 and 6 were the different approaches used in achieving the Fukui functions for the atoms in the molecule which were susceptible to electrophilic and nucleophilic attacks respectively [53]. Moreover, as shown in Table 4 and 5, the site that have highest f_k^+ , reveal the site that will possibly have nucleophilic attack whereas the site that have highest f_k^- also show the site that may be open to electrophilic attack. Therefore, the preferred site for nucleophilic and electrophilic attacks were C14 (0.023) and C1 (0.028) for **P1**, while for **P2**, the utmost value for f_k^+ was found on C6 with 0.023, and for f_k^- is found on C3 with 0.0394.

4. CONCLUSION

In this work, several descriptors (E_{HOMO} , E_{LUMO} , $\Delta E_{\text{HOMO-LUMO}}$ (energy gap), chemical hardness (η), chemical potential (μ), the fraction of electron transferred (ΔN) and (ω)) were obtained using Density Functional theory via B3LYP/6-31G** method in water for Triphenylimidazole derivatives. Several descriptors like Chemical potential, area, volume, molecular weight, ovality, PSA, polarizability, HBA and HBD increases as the % IE increase while only global nucleophilicity and log P decreases with increasing % IE. More so, the protonated molecules offered lower band gap and greater stability than the neutral molecules. Thus, low band gaps together with structural steadiness should help the adsorption of protonated species on the surface of metal.

REFERENCES

- [1] E. Osarolube, Nig. J. Phys. 10 (1998) 133.
- [2] D. S. Clark, W. R. Varney, Physical Metallurgy for Engineers. Van Nostrand Reinhold 28 Ltd., Canada (1987).
- [3] P. A. Schweitzer, Fundamentals of metallic corrosion: atmospheric and media corrosion 30 of metals. CRC Press, Taylor & Francis Group, second ed. Boca Raton, FL. (2007).
- [4] Y. El Kacimi, R. Tourir, M. Galai, R. A. Belakhmima, A. Zarrouk, K. Alaoui, M. Harcharras, H. El Kafssaoui, and M. Ebn Touhami, J. Mater. Environ. Sci. 7 (2016) 371.
- [5] S. B. Ulaeto, U. J. Ekpe, M. A. Chidiebere, and E. E. Oguzie, Int. J. Mat. Chem. 2 (2012) 158.

- [6] M. O. Abdulazeez, A. K. Oyebamiji, and B. Semire, *Lebanese Sci. J.* 17 (2016) 217.
- [7] M. Galai, M. Rbaa, Y. El Kacimi, M. Ouakki, N. Dkhirech, R. Tourir, B. Lakhri, and M. E. Touhami, *Anal. Bioanal. Electrochem.* 9 (2017) 80.
- [8] A. K. Jain, R. K. Agrawal, V. Ravichandran, and S. Sisodiya, *Asian Pacif. J. Tropic. Med.* 7 (2010) 271.
- [9] A. M. Vijesh, M. Arun, S. Telkar, S. K. Peethambar, S. Rai, and N. Isloor *European J. Med. Chem.* 46 (2011) 3531.
- [10] D. Olender, Z. Justyna, L. Victor, L. Roman, K. Aleksandra, F. Andrzej, and Z. Lucjusz, *Europ. J. Med. Chem.* 44 (2009) 645.
- [11] L. Nagarapu, A. Satyender, B. Rajashaker, K. Srinivas, P. R. Rani, K. Radhika, and G. Subhashini, *Bioorg. Med. Chem. Lett.* 18 (2008) 1167.
- [12] A. Yasodha, A. Sivakumar, G. Arunachalam, and A. Puratchikody, *J. Pharm. Sci. Res.* 1 (2009) 127.
- [13] R. Ramachandran, M. Rani, S. Senthana, and S. Kabilan, *Europ. J. Med. Chem.* 46 (2011) 1926.
- [14] S. Yadav, S. M. Patil, and B. K. Mishra, *Int. J. Drug Discovery Herbal Res. (IJDDHR)* 1 (2011) 27.
- [15] T. Hussain, H. L. Siddiqui, M. Z. Rehman, M. M. Yasin, and M. Parvez, *Europ. J. Med. Chem.* 44 (2009) 4654.
- [16] V. Padmavathi, C. Prema kumara, B. C. Venkatesh, and A. Padmaja, *Europ. J. Med. Chem.* 46 (2011) 5317.
- [17] M. Amir, I. Ahsan, W. Akhtar, S. A. Khan, and I. Ali, *Indian J. Chem.* 50B (2011) 207.
- [18] A. Puratchikody, and D. Mukesh, *Bioorg. Med. Chem.* 17 (2007) 1083.
- [19] M. Mader, A. Dios, C. Shih, R. Bonjouklian, and L. Tiechao, *Bioorg. Med. Chem. Lett.* 18 (2008) 179.
- [20] T. E. Barta, M. A. Stealey, P. W. Collins, and R. M. Weier, *Bioorg. Med. Chem. Lett.* 8 (1998) 3443.
- [21] T. Harsha, S. T. Krishnanand, A. Laxmi, and J. Chandrashekar, *Biolog. Chem. Sci.* 1 (2010) 23.
- [22] M. G. Valverde, and T. Torroba, *Molecules* 10 (2005) 318.
- [23] E. G. Brown, *Ring Nitrogen and Key Biomolecules*; Kluwer Academic Press: U.K. 31 (Chapter 2) (1998).
- [24] B. Forte, B. Malgesini, C. Piutti, F. Quartieri, A. Scolaro, and G. A. Papeo, *Drugs* 7 (2009) 705.
- [25] O. Sikemi, O. Abel Kolawole, and S. Banjo, *Manila J. Sci.* 10 (2017) 44.
- [26] E. Kraka, and D. Cremer, *J. Am. Chem. Soc.* 122 (2000) 8245.
- [27] G. Gece, and S. Bilgic, *Corros. Sci.* 52 (2010) 3304.
- [28] K. F. Khaled, *Corros. Sci.* (2010) 2905.

- [29] L. Lukovitis, A. Shaban, and E. Kalman, *Russ. J. Electrochem.* 19 (2003) 177.
- [30] B. Semire, and A. O. Odunola, *Khimiya* 22 (2013) 893.
- [31] C. Hansch, *Acc Chem. Res.* 2 (1969) 232.
- [32] C. A. Ramsden, *Quantitative Drug Design of comprehensive Medicinal Chemistry*, Oxford, Vol. 4. (1990)
- [33] P. Perez, R. Contreras, A. Vela, and O. Tapia, *Chem. Phys. Lett.* 169 (2007) 419.
- [34] P. Geerlings, F. De Proft, and W. Langenaeker, *Chem. Rev.* 103 (2003) 1793.
- [35] P. Senet, *Chem. Phys. Lett.* 275 (1997) 527.
- [36] P. Udhayakala, T. V. Rajendiran, and S. Gunasekaran, *J. Comput. Methods Mol. Des.* 2 (2012) 1.
- [37] A.Y. Musa, A. A. H. Kadhum, A. B Mohamad, A. A. B. Rahoma, and H. Mesmari, *J. Mol. Struct.* 969 (2010) 233.
- [38] Z. Zhou, and H. V. Navangul, *J. Phys. Org. Chem.* 3 (1990) 784.
- [39] S. Xia, M. Qiu, L. Yu, F. Liu, and H. Zhao, *Corros. Sci.* 50 (2008) 2021.
- [40] A. K. Singh, and M. A. Quraishi, *Int. J. Electrochem. Sci.* 7 (2012) 3222.
- [41] C. Verma, E. E. Ebenso, L. O. Olasunkanmi, M. Ahmad Quraishi, and I. Basse Obot, *J. Phys. Chem. C* 120 (2016) 11598.
- [42] S. Ramkumar, and D. Nalini, *Orient. J. Chem.* 31 (2015) 1057.
- [43] E. E. Ebenso, T. Arslan, F. Kandemirli, N. Caner, I. Love, *Int. J. Quantum. Chem.* 110 (2010) 1003.
- [44] N. O. Eddy, *Int. J. Electrochem. Sci.* 39 (2010) 288.
- [45] I. Danaee, O. Ghasemi, G. R. Rashed, M. Rashvand Awei, M. H. Maddahy *J. Mol. Struct.* 1035 (2013) 247.
- [46] K. Ramya, R. Mohan, K. K. Anupama, and A. Joseph, *Mater. Chem. Phys.* 149 (2015) 632.
- [47] G. Breke, E. Hur, and C. Ogretir, *J. Mol. Struct. (Theochem).* 578 (2002) 79.
- [48] B. Gomez, N. V. Likhanova, M. A. Dominguez-Aguilar, R. Martinez-Palou, A. Vela, and J. Gasquez, *J. Phys. Chem.* 110 (2006) 8928.
- [49] K. Fukui, T. Yonezawa, and H. Shingu, *J. Chem. Phys.* 20 (1952) 722.
- [50] I. Lukovit, E. Kalman, F. Zucchi, *Corrosion Sci.* 57 (2001) 3.
- [51] B. Semire, and A. O. Odunola, *Chem. Bulgarian J. Sci. Edu.* 22 (2013) 893.
- [52] M. Mwacham, M. Kabanda, C. M. Lutendo, and E. E. Eno, *Int. J. Electrochem. Sci.* 7 (2012) 7179.
- [53] P. Fuentealba, P. Perez, and R. Contreras, *J. Chem. Phys.* 113 (2000) 2544.