Journal of Bio- and Tribo-Corrosion (2018) 4:69
https://doi.org/10.1007/s40735-018-0185-5

Investigation of DNA–RNA Molecules for the Efficiency and Activity of Corrosion Inhibition by DFT and Molecular Docking

Burak Tüzün[1] · **Cemal Kaya**[1]

Received: 23 May 2018 / Revised: 10 September 2018 / Accepted: 12 September 2018 / Published online: 20 September 2018

Abstract
DNA and RNA molecules consist of five molecules. The activity and corrosion inhibition properties of these five molecules namely guanine, adenine, cytosine, thymine, uracil were performed by quantum chemical calculation and molecular docking. All different parameter such as E_{HOMO}, E_{LUMO}, ΔE (HOMO–LUMO energy gap), electronegativity, chemical potential, chemical hardness, electrophilicity, nucleophilicity, global softness, and proton affinity have been calculated and discussed. The interaction between studied molecules and B-DNA dodecamer is examined to find the activity of studied molecules in molecular docking calculations. Activity and corrosion inhibition ranking of studied compounds followed the order: guanine > adenine > cytosine > thymine > uracil and this ranking obtained is consistent with the experimental data.

Keywords Corrosion inhibition · Activity · DNA–RNA molecules · Docking · DFT

1 Introduction

Every organism takes place cells in the world; all multicellular organisms have a cell and a cell nucleus. This nucleus includes the DNA, the hereditary material. DNA is short for deoxyribonucleic acid. In every nucleus of an organism the DNA is exactly the same in all cells. DNA consists of four different bases (nucleotides) adenine, thymine, guanine, and cytosine. Ribonucleic acid (RNA) is synthesized in the nucleus and is very similar to DNA. The synthesis of RNA also involves the use of bases, but in RNA synthesis no thymine is used but uracil is used instead.

Corrosion is a major problem in today's industry. Corrosion is an erosion of the surface of metal or metal alloys by oxidation or other chemical effects. Many methods are used to inhibit corrosion in industry. The corrosion inhibitors adsorbed on metal surfaces are p-conjugated systems and heterocyclic organic compounds [1, 2]. Many of the organic and inorganic inhibitors containing nitrogen, oxygen, sulfur, and an aromatic ring are widely used against corrosion in recently studies.

✉ Burak Tüzün
btuzun@cumhuriyet.edu.tr

[1] Science Faculty, Department of Chemistry, Cumhuriyet University, 58140 Sivas, Turkey

In the Density Functional Theory, quantum chemical parameters such as highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), electrophilicity, electronegativity, chemical potential, chemical hardness, and nucleophilicity are a very important for reactivity [3–11]. In this study, we have studied in detail the inhibition performance of five compounds, adenine, thymine, guanine, cytosine, and uracil.

The hard and soft acid–base (HSAB) method [12, 13] is a very important method in corrosion. According to HSAB method, Pearson says that "hard acids prefer to coordinate to hard bases and soft acids prefer to coordinate to soft bases". The non-polarized chemical species is described by the hard concept. As it is well-known that hetero atom-containing structures give electrons easily to metals [14]. The molecular structures of studied molecules are given in Fig. 1.

2 Computational Details

Density functional theory (DFT) is absolutely the most widely used method for the prediction of chemical reactivity of studied molecules. In this study, the input files of studied molecules were prepared with GausView 5.0.8 programs [15]. Calculations were performed by using Gaussian IA32W-G09RevA.02 and Gaussian AS64L-G09RevD.01 programs [16, 17]. A full optimization was

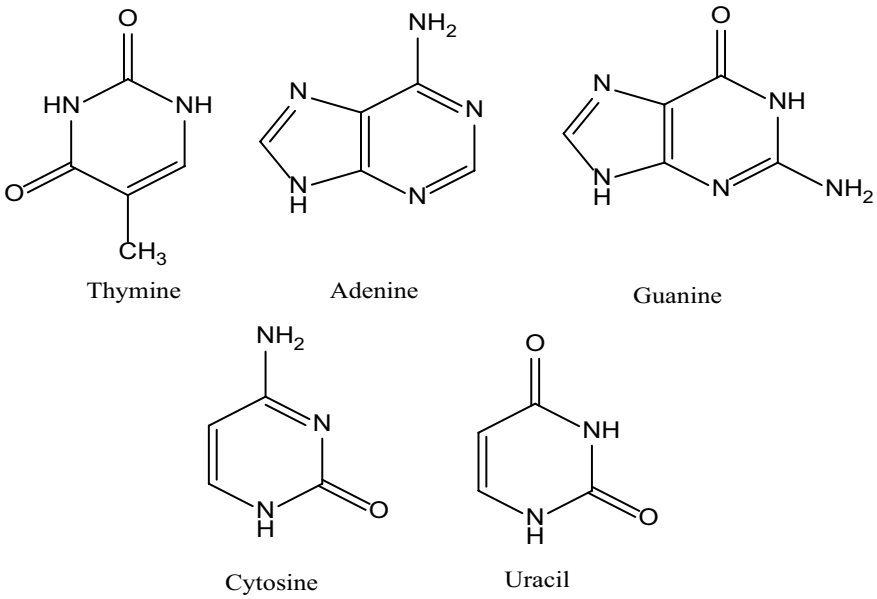

Fig. 1 The structure and schematic representation of molecules of DNA and RNA

applied using the HF and DFT/B3lyp methods with sdd, 6-31g and 6-31++g basis sets in gas and aqueous phase. With the help of this theory, the evaluation of chemical reactivity of molecules has existed a very popular in the theoretical method. Chemical reactivity descriptors include E_{HOMO}, E_{LUMO}, ΔE (HOMO–LUMO energy gap), electronegativity (χ), chemical potential (μ), chemical hardness (η), electrophilicity (ω), nucleophilicity (ε), global softness (σ), and proton affinity (PA).

$$\mu = -\chi = \left(\frac{\partial E}{\partial N}\right)_{\upsilon(r)} \tag{1}$$

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{\upsilon(r)} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right) \tag{2}$$

Electronegativity, global softness, and chemical hardness have pertained to ionization energy (I) and electron affinity (A) values of chemical molecules obtaining the following equations.

$$\chi = -\mu = \left(\frac{I + A}{2}\right) \tag{3}$$

$$\eta = \frac{I - A}{2} \tag{4}$$

It is well-known that the negative value of the highest occupied molecular orbital energy and the negative value of the lowest unoccupied molecular orbital energy were attached to the ionization energy and electron affinity, respectively ($-E_{\mathrm{HOMO}} = I$ and $-E_{\mathrm{LUMO}} = A$). on the other hand, the global softness is described as the inverse of the chemical hardness.

$$\sigma = 1/\eta \tag{5}$$

$$\chi = -\mu = \left(\frac{-E_{\mathrm{HOMO}} - E_{\mathrm{LUMO}}}{2}\right) \tag{6}$$

$$\eta = \left(\frac{E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}}{2}\right) \tag{7}$$

The global electrophilicity index (ω) presented by Parr et al. [18] is the inverse of nucleophilicity and is expressed as in Eq. (8). Electrophilicity power of studied molecules is interrelated with its global softness and electronegativity. Nucleophilicity (ε) is described as the inverse of the electrophilicity in Eq. (9).

$$\omega = \mu^2/2\eta = \chi^2/2\eta \tag{8}$$

$$\varepsilon = 1/\omega \tag{9}$$

3 Result and Discussion

3.1 Quantum Chemical Calculation

The corrosion inhibitor efficiencies of the DNA–RNA molecules were investigated by molecular docking and quantum chemical. The result obtained of these molecules indicated that studied molecules are good inhibitors. Molecular docking and quantum chemical calculations were performed

and these molecules are very active against corrosion. The obtained result of molecules is given in detail below.

In this study, quantum chemical parameters, for example, E_{HOMO}, E_{LUMO}, ΔE (HOMO–LUMO energy gap), global softness, chemical hardness, electrophilicity, nucleophilicity, proton affinity, and electronegativity are very important parameters to compare the of performances of inhibition molecules [19]. The studied molecules for protonated and non-protonated forms were investigated by quantum chemical calculation in both gas and aqueous phase and are presented in Tables 1, 2, 3, and 4.

The prediction of chemical reactivity of molecules was compared by frontier molecular orbital of studied molecules. The energy of HOMO has expressed the electron donating ability of studied molecules in Fig. 2. The molecule that has high values of energy of HOMO shows the tendency to donate the electrons of the molecule to appropriate acceptor molecules [20–27]. As a result of this theorem that the inhibition efficiencies to HOMO energy value follow the order: guanine > adenine > cytosine > thymine > uracil in all basis set. In consideration of previous explanation, energy levels of LUMO orbital of molecules are demonstrating electron accepting abilities of inhibitor molecules in Fig. 2. If the molecule has lower values of energy of LUMO, this molecule has more electron accepting ability. On the basis of the calculated LUMO energy level value given in Tables 1 and 2, the corrosion inhibition efficiency ranking of DNA-RNA molecules can be written as: guanine > adenine > cytosine > thymine > uracil.

The energy gap (ΔE) is a very important parameter for chemical reactivity of corrosion inhibitor molecules. As it is well-known, molecule that has a small energy gap value is a good corrosion inhibitor. Because the energy gap value demonstrates the binding ability of studied molecules on metal surfaces. In consideration of previous explanations, one of the studied molecules that have a high energy gap is harder compared to other molecules [20–24]. We can be seen from Tables 1 and 2, Guanine has the smallest energy gap in HF/6-31++G basis set.

Chemical hardness is described that the resistance to electron cloud polarization or deformation of chemical species. This parameter is a very important both experimental and theoretical chemistry. A chemical species tends to achieve maximum hardness. In addition, it is a measure of the stability of the chemical hardness. In quantum chemical calculations, chemical hardness, ΔE, and global softness are very important parameters that are attached to each other. According to Koopman's theorem [28], both chemical hardness value and global softness value have occurred HOMO and LUMO energy value. Soft molecules that have low HOMO–LUMO energy gap can be good corrosion inhibitor in view of the fact that soft molecules can very readily give electron of HOMO to metals [20–24]. From the light of the result given in Tables 1 and 2, we can write the corrosion inhibitor ranking of three parameter that is chemical hardness, global softness, and HOMO–LUMO energy gap value as: guanine > adenine > cytosine > thymine > uracil in HF/6-31++G basis set.

Electronegativity is a very important parameter that is a numerical value that is considered to predict the electron transfer between the metal and inhibitor [4]. Molecules having high electronegativity can't act as good corrosion inhibitor. If the molecule has a high electronegativity value, the molecule cannot be a good corrosion inhibitor [20–24]. We have calculated the value of electrons transferred from corrosion inhibitor molecule to metal (ΔN) via the following equation by Sanderson's electronegativity equalization principle [29, 30].

$$\Delta N = \frac{\chi_M - \chi_{inh}}{2(\eta_M + \eta_{inh})} \tag{10}$$

where χ_M and χ_{inh} are electronegativity of metal and electronegativity of corrosion inhibitor molecule, respectively.η_M and η_{inh} are the chemical hardness of metal and chemical hardness of corrosion inhibitor molecule, respectively. From the light of the result given in Tables 1 and 2, we have seen that guanine has the lowest electronegativity value in all basis set. Electronegativity value of corrosion inhibitor ranking follows the order: guanine > adenine > cytosine > thymine > Uracil.

In all parameters of quantum chemical calculation, we can see that guanine is the best corrosion inhibitor. On the other hand, A similar ranking was obtained in the experimental study conducted by Kassou et al. [31] who make the comparative study of low carbon steel corrosion inhibition by amino acid compounds.

3.2 Molecular Docking Calculation

The interaction between studied molecules and B-DNA dodecamer d(CGCCAATTCGCG)$_2$ (PDB code:1BNA) is examined to find the activity of studied molecules by DockingServer. In Fig. 3, molecules of guanine, adenine, cytosine, thymine, and uracil aree interacting with B-DNA dodecamer. Obtained results give information about this interaction. Many studies have been carried out on the biological activities of molecules [32, 33]. Many programs are used to study biological activities [34, 35]. Highly biologically active molecules are used as a good corrosion inhibitor. Studied DNA–RNA molecules are compared to activity using the molecular docking program.

Molecular docking is a very useful tool for obtaining an information of ligand–receptor interactions. Studied molecules are interacted with generally the upper region of 1BNA. These interactions are almost dipole–dipole

Table 1 All parameter for neutral forms of inhibitor molecules in gas phase (eV)

	E_{HOMO}	E_{LUMO}	I	A	ΔE	η	σ	χ	Pİ	ω	ε	Dipole	Energy
HF/SDD level													
Thymine	− 9.83318	2.26482	9.83318	− 2.26482	12.09801	6.04900	0.16532	3.78418	0.10460	1.18367	0.84483	5.3802	− 12279.99874
Adenine	− 8.84431	2.85803	8.84431	− 2.85803	11.70235	5.85117	0.17091	2.99314	− 1.31408	0.76556	1.30623	2.7298	− 12633.39426
Guanine	− 8.47913	3.39710	8.47913	− 3.39710	11.87623	5.93812	0.16840	2.54102	− 0.45019	0.54367	1.83934	7.6742	− 14670.32163
Cytosine	− 9.43236	2.42537	9.43236	− 2.42537	11.85773	5.92886	0.16867	3.50349	− 0.90754	1.03515	0.96605	8.2304	− 10678.25506
Uracil	− 10.24653	2.10101	10.24653	− 2.10101	12.34754	6.17377	0.16198	4.07276	0.33067	1.34338	0.74439	5.4218	− 11218.74051
HF/6-31G level													
Thymine	− 9.67508	2.65939	9.67508	− 2.65939	12.33447	6.16724	0.16215	3.50785	0.03905	0.99761	1.00240	5.2125	− 12278.16127
Adenine	− 8.65111	3.25505	8.65111	− 3.25505	11.90616	5.95308	0.16798	2.69803	− 1.38643	0.61139	1.63560	2.5842	− 12631.71977
Guanine	− 8.27722	3.72772	8.27722	− 3.72772	12.00494	6.00247	0.16660	2.27475	− 0.51041	0.43103	2.32002	7.4872	− 14668.19561
Cytosine	− 9.24269	2.84824	9.24269	− 2.84824	12.09093	6.04547	0.16541	3.19723	− 1.25987	0.84545	1.18280	7.9925	− 10676.71717
Uracil	− 10.24653	2.10101	10.24653	− 2.10101	12.34754	6.17377	0.16198	4.07276	1.87463	1.34338	0.74439	5.4218	− 11218.74051
HF/6-31++G level													
Thymine	− 9.82665	0.68083	9.82665	− 0.68083	10.50749	5.25374	0.19034	4.57291	0.10435	1.99015	0.50247	5.4107	− 12278.52444
Adenine	− 8.81846	0.91948	8.81846	− 0.91948	9.73794	4.86897	0.20538	3.94949	− 1.27285	1.60183	0.62429	2.6293	− 12632.13426
Guanine	− 8.46662	0.66043	8.46662	− 0.66043	9.12704	4.56352	0.21913	3.90310	− 0.43253	1.66912	0.59912	7.6104	− 14668.67511
Cytosine	− 9.45277	0.65063	9.45277	− 0.65063	10.10339	5.05170	0.19795	4.40107	− 4.40107	1.91712	0.52162	8.1690	− 10677.10028
Uracil	− 10.24408	0.61798	10.24408	− 0.61798	10.86205	5.43103	0.18413	4.81305	0.26400	2.13270	0.46889	5.4483	− 11217.37642
B3LYP/SDD level													
Thymine	− 6.92236	− 1.63596	6.92236	1.63596	5.28640	2.64320	0.37833	4.27916	− 0.16180	3.46384	0.28870	4.8953	− 12353.77200
Adenine	− 6.32098	− 1.06479	6.32098	1.06479	5.25619	2.62810	0.38050	3.69289	− 1.41180	2.59454	0.38542	2.6206	− 12711.80340
Guanine	− 6.00097	− 0.65417	6.00097	0.65417	5.34681	2.67340	0.37406	3.32757	− 0.81817	2.07090	0.48288	7.4580	− 14758.85084
Cytosine	− 6.47527	− 1.34643	6.47527	1.34643	5.12884	2.56442	0.38995	3.91085	0.47098	2.98211	0.33533	7.4015	− 10743.14651
Uracil	− 7.27176	− 1.80794	7.27176	1.80794	5.46382	2.73191	0.36604	4.53985	− 0.13236	3.77213	0.26510	4.9205	− 11284.67789
B3LYP/6-31G level													
Thymine	− 6.70031	− 1.29228	6.70031	1.29228	5.40803	2.70402	0.36982	3.99630	− 0.27824	2.95308	0.33863	4.5699	− 12351.72234
Adenine	− 6.07989	− 0.71349	6.07989	0.71349	5.36640	2.68320	0.37269	3.39669	− 1.51923	2.14995	0.46513	2.4798	− 12709.92890
Guanine	− 5.73104	− 0.30069	5.73104	0.30069	5.43035	2.71517	0.36830	3.01586	− 0.93230	1.67492	0.59704	7.2052	− 14756.43978
Cytosine	− 6.20533	− 0.99431	6.20533	0.99431	5.21102	2.60551	0.38380	3.59982	− 1.26262	2.48679	0.40212	7.0015	− 10741.41291
Uracil	− 7.01760	− 1.45092	7.01760	1.45092	5.56668	2.78334	0.35928	4.23426	− 0.26964	3.22077	0.31049	4.6436	− 11282.70968
B3LYP/6–31++G level													
Thymine	− 7.04536	− 1.75950	7.04536	1.75950	5.28585	2.64293	0.37837	4.40243	− 0.06452	3.66665	0.27273	4.9883	− 12352.31672
Adenine	− 6.42820	− 1.14370	6.42820	1.14370	5.28449	2.64225	0.37847	3.78595	− 1.31060	2.71235	0.36868	2.5571	− 12710.54973
Guanine	− 6.12043	− 0.91159	6.12043	0.91159	5.20884	2.60442	0.38396	3.51601	− 0.70797	2.37333	0.42135	7.4204	− 14757.18076
Cytosine	− 6.61596	− 1.46208	6.61596	1.46208	5.15388	2.57694	0.38806	4.03902	− 1.02321	3.16532	0.31592	7.4590	− 10742.01037
Uracil	− 7.38632	− 1.90835	7.38632	1.90835	5.47797	2.73898	0.36510	4.64733	− 0.02713	3.94265	0.25364	5.0010	− 11283.29617

Table 2 All parameters for neutral forms inhibitor molecules in aqueous phase (eV)

	E_{HOMO}	E_{LUMO}	I	A	ΔE	η	σ	χ	Pİ	ω	ε	Dipole	Energy
HF/SDD level													
Thymine	− 9.62774	2.43598	9.62774	− 2.43598	12.06372	6.03186	0.16579	3.59588	− 2.28197	1.07184	0.93298	7.1065	− 12280.65682
Adenine	− 8.96024	2.75300	8.96024	− 2.75300	11.71323	5.85662	0.17075	3.10362	− 3.50336	0.82236	1.21602	3.6220	− 12633.92856
Guanine	− 8.62036	3.16036	8.62036	− 3.16036	11.78072	5.89036	0.16977	2.73000	− 3.14591	0.63264	1.58068	10.2093	− 14671.30742
Cytosine	− 9.65957	2.52632	9.65957	− 2.52632	12.18590	6.09295	0.16412	3.56662	− 3.32523	1.04390	0.95795	11.1336	− 10679.15876
Uracil	− 10.00054	2.32877	10.00054	− 2.32877	12.32930	6.16465	0.16222	3.83588	− 2.04128	1.19342	0.83793	7.1404	− 11219.43264
HF/6-31G level													
Thymine	− 9.62774	2.43598	9.62774	− 2.43598	12.06372	6.03186	0.16579	3.59588	− 0.44113	1.07184	0.93298	7.1065	− 12280.65682
Adenine	− 8.96024	2.75300	8.96024	− 2.75300	11.71323	5.85662	0.17075	3.10362	− 1.86775	0.82236	1.21602	3.6220	− 12633.92856
Guanine	− 8.62036	3.16036	8.62036	− 3.16036	11.78072	5.89036	0.16977	2.73000	− 0.98057	0.63264	1.58068	10.2093	− 14671.30742
Cytosine	− 9.46664	2.90429	9.46664	− 2.90429	12.37094	6.18547	0.16167	3.28117	− 3.38951	0.87027	1.14906	10.6143	− 10677.55023
Uracil	− 10.00054	2.32877	10.00054	− 2.32877	12.32930	6.16465	0.16222	3.83588	− 0.33100	1.19342	0.83793	7.1404	− 11219.43264
HF/6-31++G level													
Thymine	− 9.63617	1.21309	9.63617	− 1.21309	10.84926	5.42463	0.18434	4.21154	− 2.25459	1.63486	0.61167	7.2718	− 12279.17651
Adenine	− 8.94663	1.21173	8.94663	− 1.21173	10.15836	5.07918	0.19688	3.86745	− 3.49193	1.47240	0.67916	3.5277	− 12632.65155
Guanine	− 8.62689	1.21990	8.62689	− 1.21990	9.84679	4.92339	0.20311	3.70350	− 3.11706	1.39293	0.71791	10.3358	− 14669.64567
Cytosine	− 9.68787	1.20493	9.68787	− 1.20493	10.89280	5.44640	0.18361	4.24147	− 3.28828	1.65156	0.60549	11.2692	− 10677.99130
Uracil	− 10.01686	1.22479	10.01686	− 1.22479	11.24166	5.62083	0.17791	4.39603	− 2.02014	1.71906	0.58171	7.2907	− 11218.06463
B3LYP/SDD level													
Thymine	− 6.79664	− 1.53501	6.79664	1.53501	5.26163	2.63082	0.38011	4.16582	− 2.44540	3.29823	0.30319	6.5375	− 12354.29990
Adenine	− 6.44616	− 1.19160	6.44616	1.19160	5.25456	2.62728	0.38062	3.81888	− 3.56274	2.77546	0.36030	3.5586	− 12712.27930
Guanine	− 6.13622	− 0.91649	6.13622	0.91649	5.21973	2.60986	0.38316	3.52635	− 3.35680	2.38234	0.41976	10.1024	− 14759.69707
Cytosine	− 6.69868	− 1.32439	6.69868	1.32439	5.37429	2.68715	0.37214	4.01153	− 3.48801	2.99433	0.33396	10.1769	− 10743.88016
Uracil	− 7.10032	− 1.65011	7.10032	1.65011	5.45021	2.72511	0.36696	4.37522	− 2.42589	3.51225	0.28472	6.5322	− 11285.22498
B3LYP/6-31G level													
Thymine	− 6.57868	− 1.20058	6.57868	1.20058	5.37810	2.68905	0.37188	3.88963	− 2.56042	2.81311	0.35548	6.0479	− 12352.18472
Adenine	− 6.21159	− 0.85254	6.21159	0.85254	5.35905	2.67953	0.37320	3.53207	− 3.67357	2.32793	0.42957	3.3381	− 12710.35621
Guanine	− 5.85920	− 0.54695	5.85920	0.54695	5.31225	2.65612	0.37649	3.20308	− 3.44510	1.93133	0.51778	9.5958	− 14757.20949
Cytosine	− 6.41486	− 0.98098	6.41486	0.98098	5.43388	2.71694	0.36806	3.69792	− 3.60105	2.51655	0.39737	9.4532	− 10742.06743
Uracil	− 6.85732	− 1.30861	6.85732	1.30861	5.54872	2.77436	0.36044	4.08296	− 2.56097	3.00441	0.33284	6.0975	− 11283.19285
B3LYP/6-31++G level													
Thymine	− 6.91365	− 1.65501	6.91365	1.65501	5.25864	2.62932	0.38033	4.28433	− 2.33979	3.49054	0.28649	6.8537	− 12352.86506
Adenine	− 6.53840	− 1.25228	6.53840	1.25228	5.28613	2.64306	0.37835	3.89534	− 3.47920	2.87047	0.34837	3.5229	− 12711.01696
Guanine	− 6.23391	− 1.05690	6.23391	1.05690	5.17701	2.58850	0.38632	3.64540	− 3.25307	2.56692	0.38957	10.3783	− 14758.03466
Cytosine	− 6.83773	− 1.42725	6.83773	1.42725	5.41048	2.70524	0.36965	4.13249	− 3.37321	3.15637	0.31682	10.6004	− 10742.75681
Uracil	− 7.21298	− 1.75406	7.21298	1.75406	5.45892	2.72946	0.36637	4.48352	− 2.31130	3.68240	0.27156	6.8163	− 11283.86672

Table 3 All parameter for protonated molecules in gas phase (eV)

	E_{HOMO}	E_{LUMO}	I	A	ΔE	η	σ	χ	ω	ε	Dipole	Energy
HF/SDD level												
Thymine	− 16.30274	− 3.19546	16.30274	3.19546	13.10728	6.55364	0.15259	9.74910	− 9.74910	7.25131	0.13791	− 12287.25414
Adenine	− 14.03710	− 2.41204	14.03710	2.41204	11.62507	5.81253	0.17204	8.22457	− 8.22457	5.81877	0.17186	− 12642.06834
Guanine	− 12.97313	− 2.14210	12.97313	2.14210	10.83103	5.41552	0.18465	7.55761	− 7.55761	5.27351	0.18963	− 14678.13182
Cytosine	− 13.90785	− 2.85450	13.90785	2.85450	11.05335	5.52668	0.18094	8.38117	− 8.38117	6.35500	0.15736	− 10686.52260
Uracil	− 15.32557	− 3.94323	15.32557	3.94323	11.38234	5.69117	0.17571	9.63440	− 9.63440	8.15489	0.12263	− 11225.76984
HF/6-31G level												
Thymine	− 16.21811	− 3.01178	16.21811	3.01178	13.20633	6.60317	0.15144	9.61495	− 9.61495	7.00022	0.14285	− 12285.48223
Adenine	− 13.88989	− 2.21530	13.88989	2.21530	11.67459	5.83730	0.17131	8.05259	− 8.05259	5.55431	0.18004	− 12640.46620
Guanine	− 12.84360	− 1.97339	12.84360	1.97339	10.87022	5.43511	0.18399	7.40849	− 7.40849	5.04919	0.19805	− 14676.06602
Cytosine	− 13.89261	− 3.17478	13.89261	3.17478	10.71783	5.35892	0.18660	8.53369	− 8.53369	6.79465	0.14717	− 10685.33704
Uracil	− 15.24394	− 3.73398	15.24394	3.73398	11.50996	5.75498	0.17376	9.48896	− 9.48896	7.82281	0.12783	− 11224.22588
HF/6-31++G level												
Thymine	− 16.25131	− 3.19981	16.25131	3.19981	13.05150	6.52575	0.15324	9.72556	− 9.72556	7.24718	0.13798	− 12285.78009
Adenine	− 13.96037	− 2.78266	13.96037	2.78266	11.17771	5.58885	0.17893	8.37151	− 8.37151	6.26982	0.15949	− 12640.76711
Guanine	− 12.92687	− 3.51275	12.92687	3.51275	9.41413	4.70706	0.21245	8.21981	− 8.21981	7.17701	0.13933	− 14676.46764
Cytosine	− 11.34724	− 6.77705	11.34724	6.77705	4.57019	2.28509	0.43762	9.06214	− 9.06214	17.96916	0.05565	− 10751.65443
Uracil	− 15.28448	− 3.94187	15.28448	3.94187	11.34261	5.67131	0.17633	9.61318	− 9.61318	8.14744	0.12274	− 11224.47242
B3LYP/SDD level												
Thymine	− 12.82483	− 7.35693	12.82483	7.35693	5.46790	2.73395	0.36577	10.09088	− 10.09088	18.62248	0.05370	− 12361.29380
Adenine	− 11.49119	− 6.29676	11.49119	6.29676	5.19442	2.59721	0.38503	8.89398	− 8.89398	15.22841	0.06567	− 12720.57520
Guanine	− 10.63565	− 6.03254	10.63565	6.03254	4.60311	2.30156	0.43449	8.33410	− 8.33410	15.08917	0.06627	− 14767.02902
Cytosine	− 11.18805	− 6.56017	11.18805	6.56017	4.62788	2.31394	0.43216	8.87411	− 8.87411	17.01641	0.05877	− 10750.03553
Uracil	− 12.65720	− 8.00538	12.65720	8.00538	4.65182	2.32591	0.42994	10.33129	− 10.33129	22.94490	0.04358	− 11292.17026
B3LYP/6-31G level												
Thymine	− 12.70455	− 7.16182	12.70455	7.16182	5.54273	2.77137	0.36083	9.93319	− 9.93319	17.80137	0.05618	− 12359.36058
Adenine	− 11.34261	− 6.08887	11.34261	6.08887	5.25374	2.62687	0.38068	8.71574	− 8.71574	14.45904	0.06916	− 12718.80813
Guanine	− 10.45524	− 5.82519	10.45524	5.82519	4.63005	2.31503	0.43196	8.14021	− 8.14021	14.31152	0.06987	− 14764.73208
Cytosine	− 11.18805	− 6.56017	11.18805	6.56017	4.62788	2.31394	0.43216	8.87411	− 8.87411	17.01641	0.05877	− 10750.03553
Uracil	− 12.52278	− 7.78823	12.52278	7.78823	4.73455	2.36727	0.42243	10.15551	− 10.15551	21.78335	0.04591	− 11290.33932
B3LYP/6-31++G level												
Thymine	− 12.90891	− 7.37979	12.90891	7.37979	5.52913	2.76456	0.36172	10.14435	− 10.14435	18.61195	0.05373	− 12359.74124
Adenine	− 11.58860	− 6.29323	11.58860	6.29323	5.29538	2.64769	0.37769	8.94092	− 8.94092	15.09618	0.06624	− 12719.22033
Guanine	− 10.68219	− 6.06547	10.68219	6.06547	4.61672	2.30836	0.43321	8.37383	− 8.37383	15.18848	0.06584	− 14765.24872
Cytosine	− 11.01961	− 6.63065	11.01961	6.63065	4.38896	2.19448	0.45569	8.82513	17.74519	0.05635	9.5715	− 11819.42107
Uracil	− 12.68523	− 8.01246	12.68523	8.01246	4.67278	2.33639	0.42801	10.34884	22.91969	0.04363	2.6950	− 11290.68330

Table 4 All parameter for protonated molecules in aqueous phase (eV)

	E_{HOMO}	E_{LUMO}	I	A	ΔE	η	σ	χ	ω	ε	Dipole	Energy
HF/SDD level												
Thymine	− 11.92820	1.01146	11.92820	− 1.01146	12.93966	6.46983	0.15456	5.45837	− 5.45837	2.30252	0.43431	− 12290.29879
Adenine	− 10.34748	1.33636	10.34748	− 1.33636	11.68384	5.84192	0.17118	4.50556	− 4.50556	1.73745	0.57556	− 12644.79192
Guanine	− 9.69767	1.84223	9.69767	− 1.84223	11.53990	5.76995	0.17331	3.92772	− 3.92772	1.33684	0.74803	− 14681.81333
Cytosine	− 10.18367	1.11976	10.18367	− 1.11976	11.30343	5.65171	0.17694	4.53196	− 4.53196	1.81703	0.55035	− 10689.84399
Uracil	− 10.89226	0.46205	10.89226	− 0.46205	11.35431	5.67716	0.17614	5.21510	− 5.21510	2.39533	0.41748	− 11228.83392
HF/6-31G level												
Thymine	− 11.85800	1.18588	11.85800	− 1.18588	13.04388	6.52194	0.15333	5.33606	− 5.33606	2.18290	0.45811	− 12288.45795
Adenine	− 10.22857	1.53283	10.22857	− 1.53283	11.76140	5.88070	0.17005	4.34787	− 4.34787	1.60729	0.62217	− 12643.15632
Guanine	− 9.55726	2.02209	9.55726	− 2.02209	11.57935	5.78968	0.17272	3.76758	− 3.76758	1.22586	0.81575	− 14679.64800
Cytosine	− 10.05877	1.36112	10.05877	− 1.36112	11.41989	5.70995	0.17513	4.34882	− 4.34882	1.65608	0.60384	− 10688.29973
Uracil	− 10.81280	0.67403	10.81280	− 0.67403	11.48683	5.74342	0.17411	5.06939	− 5.06939	2.23723	0.44698	− 11227.12365
HF/6-31++G level												
Thymine	− 11.90045	0.93445	11.90045	− 0.93445	12.83490	6.41745	0.15583	5.48300	− 5.48300	2.34231	0.42693	− 12288.79111
Adenine	− 10.30231	1.03976	10.30231	− 1.03976	11.34207	5.67103	0.17633	4.63128	− 4.63128	1.89108	0.52880	− 12643.50348
Guanine	− 9.68597	0.97118	9.68597	− 0.97118	10.65715	5.32858	0.18767	4.35739	− 4.35739	1.78161	0.56129	− 14680.12273
Cytosine	− 10.19918	1.02778	10.19918	− 1.02778	11.22696	5.61348	0.17814	4.58570	− 4.58570	1.87305	0.53389	− 10688.63958
Uracil	− 10.87648	0.40572	10.87648	− 0.40572	11.28220	5.64110	0.17727	5.23538	− 5.23538	2.42942	0.41162	− 11227.44477
B3LYP/SDD level												
Thymine	− 8.90799	− 3.22457	8.90799	3.22457	5.68341	2.84171	0.35190	6.06628	− 6.06628	6.47494	0.15444	− 12364.10530
Adenine	− 8.01246	− 2.58701	8.01246	2.58701	5.42545	2.71272	0.36863	5.29973	− 5.29973	5.17693	0.19316	− 12723.20204
Guanine	− 7.28101	− 2.19570	7.28101	2.19570	5.08530	2.54265	0.39329	4.73836	− 4.73836	4.41508	0.22650	− 14770.41387
Cytosine	− 7.55965	− 2.80225	7.55965	2.80225	4.75740	2.37870	0.42040	5.18095	− 5.18095	5.64221	0.17724	− 10754.72818
Uracil	− 8.25518	− 3.64908	8.25518	3.64908	4.60611	2.30305	0.43421	5.95213	− 5.95213	7.69149	0.13001	− 11295.01087
B3LYP/6-31G level												
Thymine	− 8.75560	− 3.01205	8.75560	3.01205	5.74355	2.87178	0.34822	5.88383	− 5.88383	6.02753	0.16591	− 12362.10514
Adenine	− 7.84129	− 2.37067	7.84129	2.37067	5.47062	2.73531	0.36559	5.10598	− 5.10598	4.76565	0.20983	− 12721.38977
Guanine	− 7.07910	− 1.97094	7.07910	1.97094	5.10816	2.55408	0.39153	4.52502	− 4.52502	4.00844	0.24947	− 14768.01459
Cytosine	− 7.36564	− 2.56252	7.36564	2.56252	4.80312	2.40156	0.41640	4.96408	− 4.96408	5.13043	0.19492	− 10753.02848
Uracil	− 8.11232	− 3.41778	8.11232	3.41778	4.69455	2.34727	0.42603	5.76505	− 5.76505	7.07966	0.14125	− 11293.11382
B3LYP/6-31++G level												
Thymine	− 8.96785	− 3.27954	8.96785	3.27954	5.68831	2.84416	0.35160	6.12370	− 6.12370	6.59241	0.15169	− 12362.56485
Adenine	− 8.10307	− 2.59599	8.10307	2.59599	5.50708	2.75354	0.36317	5.34953	− 5.34953	5.19648	0.19244	− 12721.85615
Guanine	− 7.35475	− 2.22074	7.35475	2.22074	5.13401	2.56701	0.38956	4.78774	− 4.78774	4.46483	0.22397	− 14768.64772
Cytosine	− 7.63830	− 2.83899	7.63830	2.83899	4.79931	2.39965	0.41673	5.23864	− 5.23864	5.71819	0.17488	− 10753.49002
Uracil	− 8.29954	− 3.68363	8.29954	3.68363	4.61590	2.30795	0.43328	5.99159	− 5.99159	7.77726	0.12858	− 11293.53802

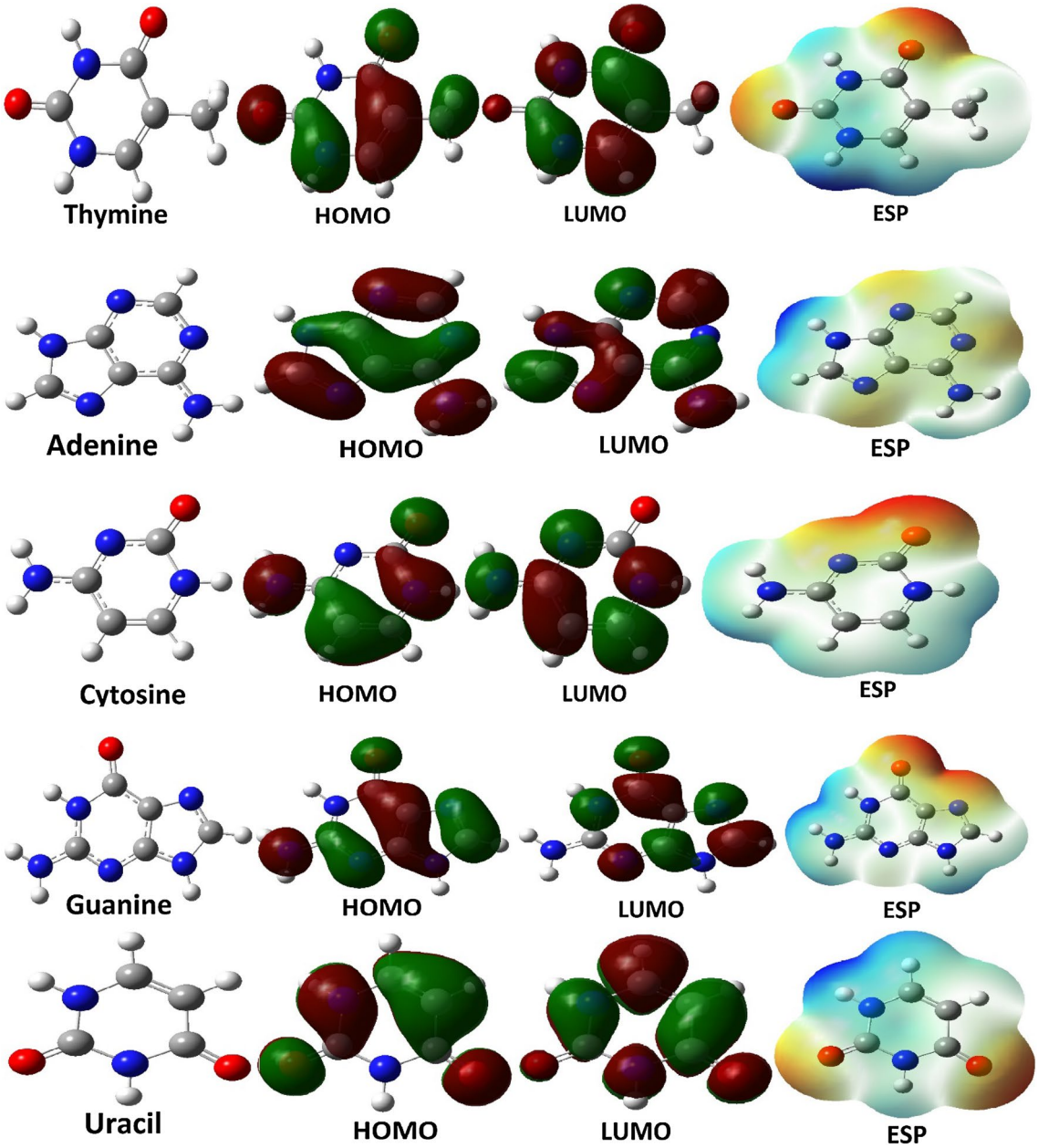

Fig. 2 Structures of HOMO, LUMO, and ESPs of molecules of DNA and RNA

interactions. For each interaction, heteroatoms increase the biological reactivity of these molecules.

In Table 5, we can see that interaction energies are formed when molecules bind to the protein. According to obtained results for molecules, inhibition constant is 1.70, 2.90, 10.21, 11.37, and 11.29 for guanine, adenine, thymine, cytosine, and uracil, respectively. Value of Ki gives information that both molecules can inhibit an enzyme and molecules can interact with a substrate for the enzyme. If Ki has bigger value, the extra drug is needed to inhibit the enzyme activity. The vdW, hydrogen bond, and dissolved energy are the numerical value of the position the molecule receives relative to the target protein. vdW, hydrogen bond, and dissolved energy have negative value, the molecule is well-bonded to an active site on the protein. In addition, the electrostatic energy has a negative value, and this value shows that the molecule is linked to a protein [25].

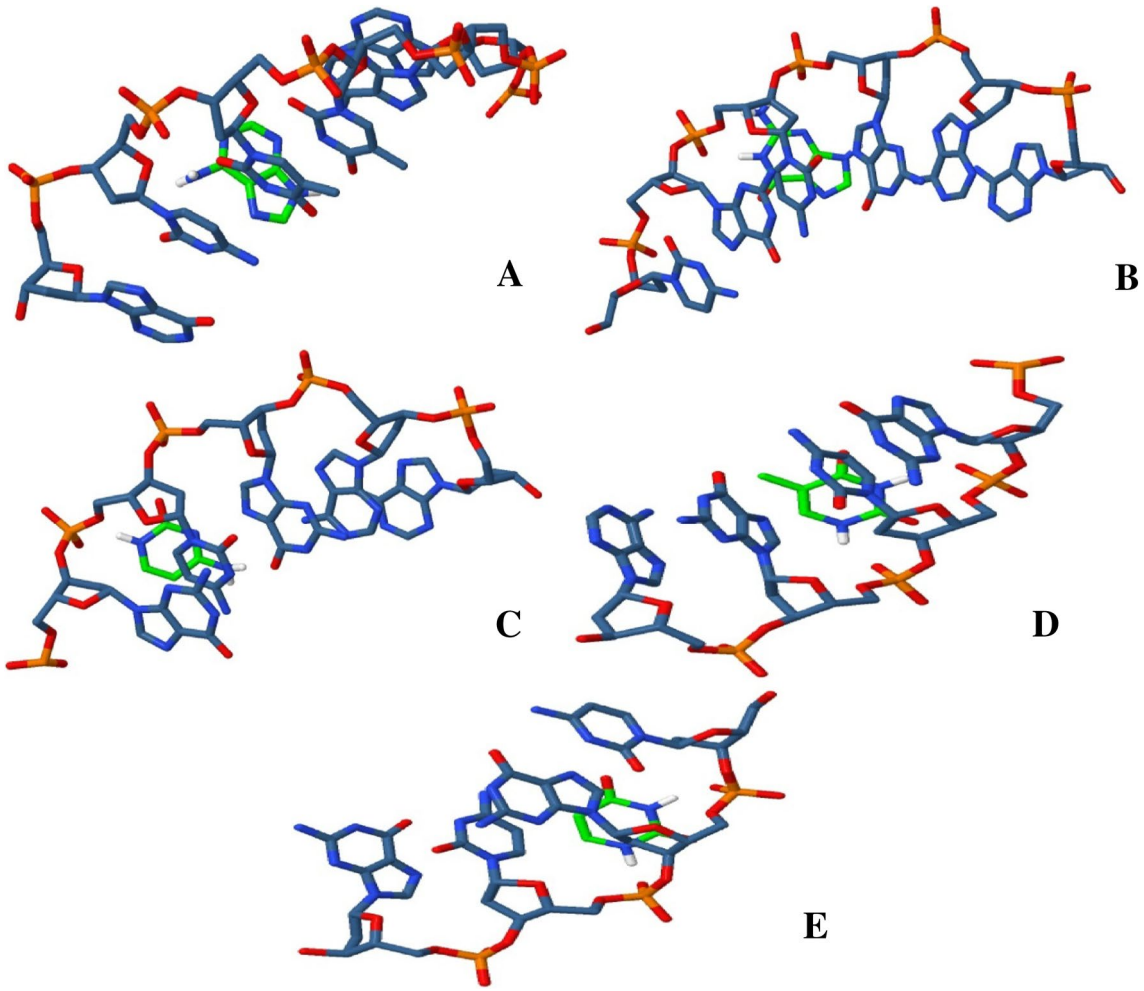

Fig. 3 Interactions between protein and adenine (**a**), guanine (**b**), cytosine (**c**), thymine (**d**), and uracil (**e**)

Table 5 Molecular docking energy data for studies molecule

	Guanine	Adenine	Thymine	Cytosine	Uracil
Est. free energy of binding (kcal/mol)	− 3.77	− 3.46	− 2.72	− 2.65	− 2.66
Est. inhibition constant (Ki/mM)	1.71	2.90	10.21	11.37	11.29
vdW + Hbond + desolv energy (kcal/mol)	− 3.16	− 3.52	− 2.39	− 2.76	− 2.18
Electrostatic energy (kcal/mol)	− 0.62	− 0.24	− 0.33	− 0.19	− 0.47
Total intermolec. energy (kcal/mol)	− 3.77	− 3.76	− 2.72	− 2.95	− 2.66
Frequency (%)	10	60	20	20	70
Interact. surface	294.965	263.254	267.128	250.532	243.590

4 Conclusions

From the light of the the result given in this paper, quantum chemical parameters and results of molecular docking give information about inhibition of studied molecule. Parameters such as HOMO, LUMO, and ΔE (HOMO–LUMO energy gap) demonstrate which molecule is the better inhibitor. Results of molecular docking give information about molecular activity. The molecule with the higher molecular activity is the better inhibitor. in quantum chemical calculation, studied molecules are investigated in different basis sets that show how molecule activity is affected. Results of molecular docking give six parameters that offer knowledge about molecular inhibition. In quantum chemical calculations, the neutral and protonated forms are studied in gas and aqueous phases. In this study, following obtained results are presented.

1. The results of quantum chemical calculation and molecular docking calculations showed that the corrosion inhibition ranking of DNA–RNA molecules can be presented as: guanine > adenine > cytosine > thymine > uracil.
2. The obtained different parameters of molecular docking software show that guanine is good activity molecule against B-DNA dodecamer d(CGCCAATTCGCG)2 (PDB code:1BNA).
3. In this study, the theoretical results obtained are very important towards rational designing of new molecules as a corrosion inhibitor.

Acknowledgements This research was made possible by TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure). This work is supported by the Scientific Research Project Fund of Cumhuriyet University under the project number F-544.

References

1. Obot IB, Macdonalda DD, Gasema ZM (2015) Density functional theory (DFT) as a powerful tool for designing new organic corrosion inhibitors. Part 1: an overview. Corros Sci 99:1–30
2. Leçe HD, Emregül KC, Atakol O (2015) Difference in the inhibitive effect of some Schiff base compounds containing oxygen, nitrogen and sulfur donors. Corros Sci 50:1460–1468
3. Kaya S, Banerjee P, Saha SK, Tüzün B, Kaya C (2016) Theoretical evaluation of some benzotriazole and phospono derivatives as aluminum corrosion inhibitors: DFT and molecular dynamics simulation approaches. RSC Adv 6:74550–74559
4. Kaya S, Tüzün B, Kaya C, Obot IB (2016) Determination of corrosion inhibition effects of amino acids: quantum chemical and molecular dynamic simulation study. J Taiwan Inst Chem Eng 58:528–553
5. Kaya S, Kaya C, Guo L, Kandemirli F, Tüzün B, Uğurlu İ, Madkour L, Saraçoğlu M (2016) Quantum chemical and molecular dynamics simulation studies on inhibition performances of some thiazole and thiadiazole derivatives against corrosion of iron. J Mol Liq 219:497–504
6. Obot IB, Kaya S, Kaya C, Tüzün B (2016) Density functional theory (DFT) modeling and Monte Carlo simulation assessment of inhibition performance of some carbohydrazide Schiff bases for steel corrosion. Phys E 80:82–90
7. Obot IB, Kaya S, Kaya C, Tüzün B (2016) Theoretical evaluation of triazine derivatives as steel corrosion inhibitors: DFT and Monte Carlo simulation approaches. Res Chem Intermed 42(5):4963–4983
8. Tüzün B (2014) Selectivity of salicylaldoxime and its derivatives. J New Results Sci 3(5):67–85
9. Kaya S, Guo L, Kaya C, Tüzün B, Obot IB, Touir R, Islam N (2016) Quantum chemical and molecular dynamic simulation studies for the prediction of inhibition efficiencies of some piperidine derivatives on the corrosion of iron. J Taiwan Inst Chem Eng 65:522–529
10. Kaya S, Tüzün B, Kaya C (2017) Conceptual density functional theoretical investigation of the corrosion inhibition efficiencies of some molecules containing mercapto (-SH) group. Curr Phys Chem 7(2):147–153
11. Hepokur C, Günsel A, Yarasir MN, Bilgiçli AT, Tüzün B, Tüzün G, Yaylim I (2017) Novel type ketone-substituted metallophthalocyanines: synthesis, spectral, structural, computational and anticancer studies. RSC Adv 89:56296–56305
12. Pearson RG (1963) Hard and soft acids and bases. J Am Chem Soc 85:3533–3539
13. Pearson RG (1968) Hard and soft acids and bases, HSAB, part 1: fundamental principles. J Chem Educ 45:581–587
14. Pearson RG (1997) Chemical hardness: applications from molecules to solids. Wiley-VCH: Weinheim
15. Dennington RD, Keith TA, Millam JM (2009) GaussView 5.0. Gaussian Inc, Wallingford CT
16. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2009) Gaussian 09, revision D.01. Gaussian Inc, Wallingford CT
17. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2009) Gaussian 09, Revision A.02. Gaussian Inc, Wallingford CT
18. Parr RG, Yang W (1989) Density functional theory of atoms and molecules. Oxford University Press, Oxford
19. Albrakaty RH, Wazzan NA, Obot IB (2018) Theoretical study of the mechanism of corrosion inhibition of carbon steel in acidic solution by 2-aminobenzothaizole and 2-mercatobenzothiazole. Int J Electrochem Sci 13:3535–3554
20. Tüzün B (2018) Theoretical evalution of six indazole derivatives as corrosion inhibitors based on dft. Turk Comput Theor Chem 2(1):12–22
21. Alaoui K, Touir R, Galai M, Serrar H, Ouakki M, Kaya S, Tüzün B, Boukhris S, Ebn Touhami M, El Kacimi Y (2018) Electrochemical and computational studies of some triazepine carboxylate compounds as acid corrosion inhibitors for mild steel. J Bio-Tribo-Corros 4:37
22. Guo L, Safi ZS, Kaya S, Shi W, Tüzün B, Altunay N, Kaya C (2018) Anticorrosive effects of some thiophene derivatives against the corrosion of iron: a computational study. Front Chem 6:155–166
23. Üngördü A, Tezer N (2017) DFT study on metal-mediated uracil base pair complexes. J Saudi Chem Soc 21(7):837–844
24. Üngördü A, Tezer N (2017) The solvent (water) and metal effects on HOMO-LUMO gaps of guanine base pair: a computational study. J Mol Graph Model 74:265–272

25. Üngördü A, Tezer N (2017) Effect on frontier molecular orbitals of substituents in 5-position of uracil base pairs in vacuum and water. J Theor Comput Chem 16(07):1750066
26. Madkour LH, Kaya S, Obot IB (2018) Computational, Monte Carlo simulation and experimental studies of some arylazotriazoles (AATR) and their copper complexes in corrosion inhibition process. J Mol Liq 260:351–374
27. Sayın K, Üngördü A (2018) Investigation of anticancer properties of caffeinated complexes via computational chemistry methods. Spectrochim Acta Part A Mol Biomol Spectrosc 193:147–155
28. Koopmans T (1933) Ordering of wave functions and eigen-energies to the individual electrons of an atom. Physica 1:104–113
29. Sanderson RT (1976) Chemical bond and bond energy. Academic Press, New York
30. Sanderson RT (1954) Electronegativities in inorganic chemistry. J Chem Educ 31:2–7
31. Kassou O, Galai M, Ballakhmima RA, Dkhireche N, Rochdi A, Touhami ME, Touir R, Zarrouk A (2015) Comparative study of low carbon steel corrosion inhibition in 200 ppm NaCl by aöino acid compounds. J Mater Environ Sci 6(4):1147–1155
32. Sayın K, Karakaş D (2018) Quantum chemical investigation of levofloxacin-boron complexes: a computational approach. J Mol Struct 1158:57–65
33. Sayın K, Karakaş D (2018) Computational investigations of trans–platinum(II) oxime complexes used as anticancer drug. Spectrochim Acta Part A Mol Biomol Spectrosc 188:537–546
34. Özalp A, Yavuz S, Sabancı N, Çopur F, Kökbudak Z, Sarıpınar E (2016) 4D-QSAR investigation and pharmacophore identification of pyrrolo[2,1-c][1,4] benzodiazepines using electron conformational-genetic algorithm method. SAR QSAR Environ Res 27(4):317–342
35. Tüzün B, Yavuz S, Sarıpınar E (2018) 4D-QSAR analysis and pharmacophore modeling: propoxy methylphenyl oxasiazole derivatives by electron conformatitional-genetic algorithm method. J Phys Theor Chem 14(2):149–164