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Investigations of Solvent Effect on Electrochemical and Electronically Properties of Some Quinone Drugs: A Computational Study

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ABSTRACT

Quantum mechanics computations were performed for some quinone drugs using Gaussian 09 and density functional theory at the B3LYP/6-311G* level in liquid and in the phase of gas. The model of the polarized continuum is applied to measure solvation energies. Electrode potentials ($E°_{1/2}$), hardness index (η), chemical potential (μ), energy gap (E_g), and electrophilicity (ω) of some important quinone derivatives in three solvents with different polarities (MeOH, DMSO, and THF) have been calculated. Consequences show that this approach could be advantageous in our prognosis of the electrode potentials of molecules in various solvents. We have demonstrated that 2, 5-dimethyl-1, 4-benzoquinone is more reactive than anthraquinone and phenyl-1, 4-benzo quinone. Also, its antioxidant activity is larger than that of the other quinone-based drugs.

1. INTRODUCTION

Quinones are a series of widespread compounds in living organisms possessing a diversity of physiological and biochemical functions. They constitute a broad range of organic

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compounds with amazing properties such as antifungal, antibacterial, antitumor, antibiotical, and so on [1, 2]. Their activities originate from the reversible electron transfer behavior [3−5].

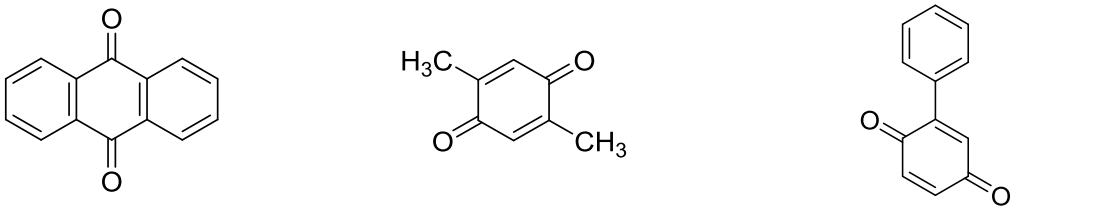
One approach to studying drugs is to apply Gaussian software and density functional theory (DFT). This theory is a computational method of quantum mechanics that benefit in chemistry and also in physics in order to explore the electron's structure of the basic state in multiple systems, especially atoms, molecules, and dense phases. It expresses the characteristics of multi-electron systems by specific functions, depending on the electron density. For this reason, the name of the functional density theory is derived from the use of functions related to electron density. DFT is the most widely used method in computational chemistry and physics [6−9]. Using a series of approximations increases the method's accuracy in the calculation of exchange-correlation interactions.

DFT calculations are much more cost-effective than conventional methods like Hartree-Fock. Also, this method is nearly the initial computational and semi-experimental computational theory, due to the Schrödinger equation being resolved assuredly. In any other way, the empirical data are researched. The theory of functional density's data processing can calculate around 500 atoms [10-15]. Thermodynamic, electronic, and orbital features of drugs can be examined by employing the Gaussian software. Through the medium of the electronic features, the drug's reactivity can be determined. Energy gap, chemical potential, chemical hardness, and electrophilicity are some of the criteria that reveal the mentioned features. The HOMO and LUMO levels of energies are used straightly in the Gaussian calculations output file.

The antioxidant activity of a compound has a connection with electrochemical parameters, particularly its oxidation potential, which supplies an approximate calculation of the energy needed to award an electron. Absolutely, the lower the oxidization potential, the more comfortably will the compound be awarded an electron and the greater will its wonted antioxidant activity be [16]. The perseverance of the oxidation potential and, normally, the examination of the electrochemical behavior of a compound can effortlessly be operated by using cyclic voltammetry. Cyclic voltammetry outcomes with those results of antioxidant protocols can be correlated [17] by cause redox behavior of an antioxidant at an electrode is linked to its behavior in a chemical redox reaction with a radical [18]. However, the potential of oxidation and, therefore, the convenience of oxidation in an electrode is affected in most situations by the solvent applied and its interactions with reactants or their intermediates [19].

In this research, Gauss View software was used to design the drugs. Then, optimization was done by using the Gaussian 09 [20] and DFT with the B3LYP method in the 6-311G* base series. DFT indicators are powerful tools to justify reactivity and region selectivity in polar organic reactions [21]. All steps described above were carried out for a gas phase and the CPCM in some selected solvents. In this work, the inherent parameters, such as electrode potentials, chemical hardness, and chemical potential, energy gap, and

electrophilicity of some important quinone derivatives, illustrated in Scheme.1, are studied in detail in three different solvents (MeOH, DMSO, and THF) having different polarity.



anthraquinone 2,5-dimethyl-1,4-benzoquinone phenyl-1,4-benzoquinone

Scheme. 1. The structure of the studied quinones-based drugs.

2. MAIN RESULTS

The vibrational frequencies of some picked quinones are computed for the structure validation on account of the molecular parameters checked by the structure. Accordingly, the standard electrode potential and other parameters of the reaction of quinones are computed by the optimized structures of the Gaussian 09 program (the results are presented in Figure 1). Nearly all investigations results have pointed out that the theory of DFT is a strong method for estimating the harmonic and geometry vibration of organic compounds [22-26]. Then, the B3lyp/6-311G* with polarized continuum model (PCM) solvation including CPCM were accomplished to gain vision into the molecular structure, solvation energies, sum of electronic, thermal free energies, and the vibrational frequencies of both diminished quinones (X) and their form of oxidized (XH_2) at the electrode.

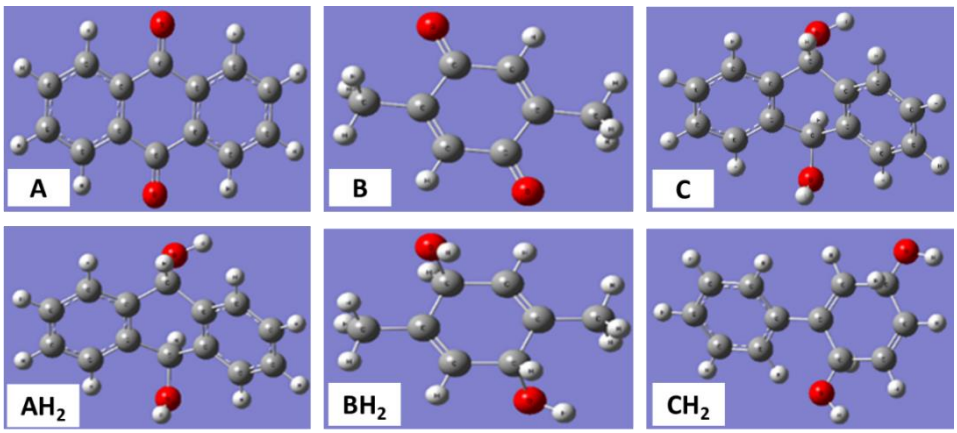


Figure 1. Optimized structures of quinone-based drugs in oxidation (ox.) and reduction (red.) state A: anthraquinone B: 2, 5-dimethyl-1, 4-benzoquinone C: phenyl-1, 4-benzoquinone.

Reaction 1 characterized the reaction of the quinones of electron oxidation (X). The quinones form (XH_2) can be transformed to its reduced form (X) by applying one of the quinones as a reference (anthraquinone=AQ), in accordance with the following reaction:

$$XH_2 + AQ \rightarrow X + AQH_2 \quad (1)$$

Geometry optimization of all compounds was performed in the solution phase and in the gas phase at the DFT/6-311G* level of theory. The Gibbs free energy, kJ mol^{-1}; transformation in the gas-phase (ΔG°_{gas}) of reaction 1 was computing applying Equation (2):

$$\Delta G^\circ_{gas} = \{G^\circ_{gas}(X) + G^\circ_{gas}(AQH_2)\} - \{G^\circ_{gas}(XH_2) + G^\circ_{gas}(AQ)\} \quad (2)$$

A usual procedure to compute Gibbs free-energy transformation of an interaction (ΔG°_{total}) is by summing ΔG°_{gas} and ΔG°_{solv} by applying the thermodynamic cycle of Figure 2 and Equation (3)

$$\Delta G^\circ_{total} = \Delta G^\circ_{gas} + \Delta G^\circ_{solv}, \quad (3)$$

$$\Delta G^\circ_{total} = G^\circ_{gas}(X) + G^\circ_{gas}(AQH_2) - G^\circ_{gas}(XH_2) + G^\circ_{gas}(AQ) + \Delta G^\circ_{solv}(X) + \Delta G^\circ_{solv}(AQH_2) - \Delta G^\circ_{solv}(X) - \Delta G^\circ_{solv}(AQ).$$

Lastly, $E^\circ_{1/2}$ is computed in accordance with Equation (4)

$$\Delta G^\circ_{total} = nF\,(E^\circ_{1/2} - E^\circ_{ref}), \quad (4)$$

where ΔG°_{total}/kJ mol^{-1} is the entire free energy for reaction 1, E°_{ref} is the experimental potential for the reference molecule (anthraquinone), $E^\circ_{1/2}$ is the computed potential and F is the Faraday constant, F=96941 C mol^{-1}.

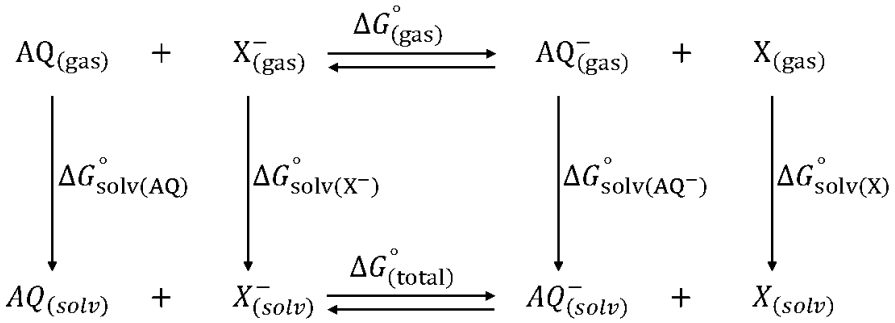


Figure 2. The thermodynamic cycle is suggested by converting the standard Gibbs energy of an isodesmic interaction in the gas phase to the standard Gibbs energy of a reaction in solution.

To attain the half-wave potential of the examined drugs first, the molecules were optimized by reduction and oxidation applying the Gaussian software. The outcomes are summarized in Figure 3. Therefore, the values of G° were attained for the oxidation and declined the solution and the gas state (see Table 1). Likewise, the ΔG° total values for each molecule were determined. In the end, the half-wave potential was computed [27].

(Table 2). It is inevitable to know the state of oxidation and decline of quinone derivatives and to obtain the Gibbs free energy values.

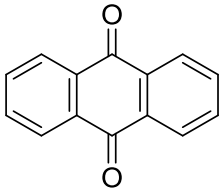
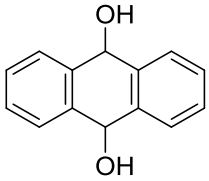
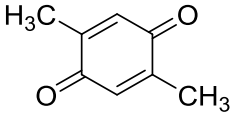
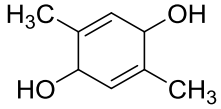
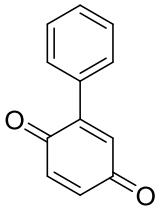
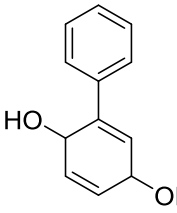
Comp.	Oxidation state	Reduction state
A		
B		
C		

Figure 3. Oxidation and reduction states of quinone derivatives.

With the following equation, the amount of chemical potential is calculated [24]. The outcomes show computation potential values for the three compounds, in the existence of MeOH, DMSO, and THF solvents close together. The value for the 2, 5-dimethyl-1, 4-benzoquinone is higher than those of the anthraquinone and phenyl-1, 4-benzoquinone. The values of $E^{o}_{1/2}$ in the three solvents follow the relation: B > C > A.

From Table 2, it is obvious that the antioxidant activity of the 2, 5-dimethyl-1, 4-benzoquinone is the largest one, while, the antioxidant activity of the anthraquinone is the smallest.

Table 1. Gibbs free energy of the examined quinone derivatives for both oxidation (X) and reduction (XH_2) forms in gas and solution phases.

	$\Delta G°$ / Hartree[1]			
Comp.	Gas phase	MeOH	DMSO	THF
A	-688.610908	-688.621208	-688.621326	-688.619922
AH_2	-690.952737	-690.966177	-690.966323	-690.964568
B	-459.972750	-459.982052	-459.982157	-459.980909
BH_2	-462.318006	-642.330706	-462.330845	-462.329177
C	-612.359481	-612.370680	-612.370809	-612.369331
CH_2	-614.467730	-614.479873	-614.480036	-614.478077

[1]1 Hartree = 2625.49975 kJ mol^{-1}.

Table 2. Solvation energies and standard electrode potentials, V; of the examined quinone derivatives in MeOH, DMSO, and THF solvents.

Comp.[1]	Solvent	ΔG^{o}_{gas} kJ/mol^{-1}	$\Delta\Delta G^{o}_{solv.}$ kJ/mol^{-1}	$\Delta G^{o}_{tot.}$ kJ/mol^{-1}	$E^{o}_{1/2}$ V
A		0.000	0.000	0.000	0.275
B	MeOH	8.998	0.677	9.675	0.325
C		10.817	-5.766	5.051	0.301
A		0.000	0.000	0.000	0.275
B	DMSO	8.998	0.693	9.691	0.325
C		10.817	-5.750	5.067	0.301
A		0.000	0.000	0.000	0.275
B	THF	8.998	0.512	9.510	0.324
C		10.817	-6.091	4.726	0.299

[1]A compound is used as a reference.

The energy gap, which is the HOMO and LUMO energy levels distinction is acquired as follows:

$$\text{ENERGY GAP} = E_{LUMO} - E_{HOMO}. \quad (5)$$

LUMO is the lowest unemployed level for electrons and HOMO is the highest employed by electrons level (see Figure 4). These energy level values are computed from the NBO result file information. The values of E_{HOMO}, E_{LUMO}, and E_g of the quinone-based drugs in solution and gas phases were computed through the B3LYP/6-311G*. The greater the diversity between the two energy levels HOMO and LUMO is, the harder the transfer of electrons between these levels due to the larger energy needed for the transfer of electrons between these two surfaces. In this way, the reactivity declined (Table 3).

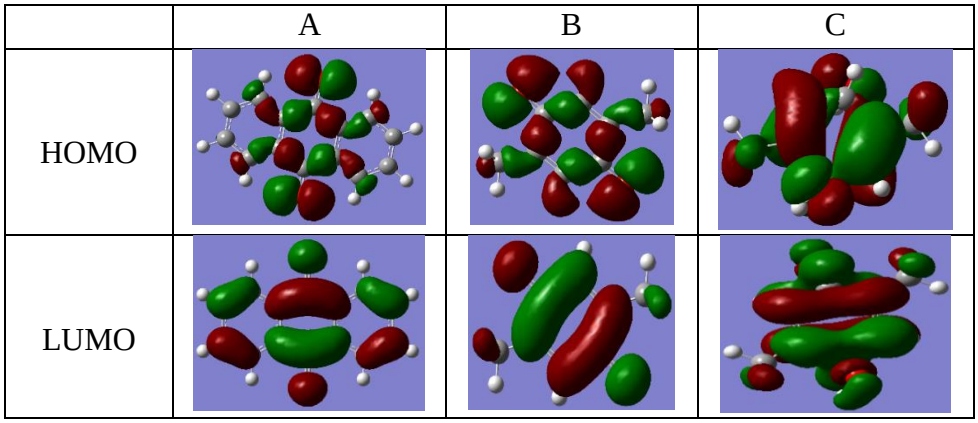


Figure 4. The HOMO and LUMO orbitals of quinone-based drugs.

Table 3. Calculated values of E_{HOMO}, E_{LUMO}, and E_g in quinone-based drugs in the gas and solution phases.

	Comp.	Gas Phase	MeOH	DMSO	THF
E_{HOMO} / eV	A	-0.27046	-0.27705	-0.27713	-0.27616
	AH_2	-0.25220	-0.25586	-0.25590	-0.25546
	B	-0.27549	-0.27861	-0.27864	-0.27825
	BH_2	-0.25150	-0.25391	-0.25394	-0.25363
	C	-0.26029	-0.25889	-0.25888	-0.25904
	CH_2	-0.23337	-0.15890	-0.15891	-0.15880
E_{LUMO} / eV	A	-0.11958	-0.12407	-0.12412	-0.12351
	AH_2	-0.03414	-0.03629	-0.03632	-0.03597
	B	-0.13789	-0.13889	-0.13889	-0.13881
	BH_2	-0.02257	-0.02130	-0.02129	-0.02138
	C	-0.14424	-0.14496	-0.14497	-0.14486
	CH_2	-0.03391	-0.03347	-0.03355	-0.03258
HLG (E_g)	A	0.15088	0.15298	0.15301	0.15265
	AH_2	0.21806	0.21957	0.21958	0.21949
	B	0.13760	0.13972	0.13975	0.13944
	BH_2	0.22893	0.23261	0.23265	0.23225
	C	0.11605	0.11393	0.11391	0.11418
	CH_2	0.19946	0.12543	0.12536	0.12622

The chemical potential (μ) value is determined from the following equation [28]:

$$\mu = -(IP+EA)/2, \quad (6)$$

where IP ($-E_{HOMO}$) is the potential of ionization and EA ($-E_{LUMO}$) is the electron closeness of the molecule. Physically, the chemical potential explains an electron's tendency to get away from a balanced system. The outcomes attained are presented in Table IV. Obviously, the absolute value of the chemical potential of the 2, 5-dimethyl-1, 4-benzoquinone is higher than those of the anthraquinone and phenyl-1, 4-benzoquinone.

In a molecule, the chemical hardness [29] calculated the protection to transformations in the electron configuration, charge, or electron transmission. Based on the energy level of the molecular orbitals, the chemical hardness corresponds to the HOMO and LUMO levels of the mean difference. The Chemical hardness values of the investigated quinone-based drugs in the gas and solution phase were calculated by the described above software and the results obtained are revealed in Table V.

Table 4. Chemical potential (μ) and Softness of quinone-based drugs in the gas and solution phase.

	μ / eV			
Composition	Gas Phase	MeOH	DMSO	THF
A	-0.19502	-0.20056	-0.20062	-0.19983
AH_2	-0.14317	-0.14607	-0.14611	-0.14571
B	-0.20669	-0.20875	-0.20876	-0.20853
BH_2	-0.13703	-0.13760	-0.13761	-0.13750
C	-0.20226	-0.20192	-0.20192	-0.20195
CH_2	-0.13364	-0.09618	-0.09623	-0.09569

The outcomes presented that in both solution phases and gas, the chemical hardness in anthraquinone is larger than of 2, 5-dimethyl-1, 4-benzoquinone, and phenyl-1, 4-benzoquinone. There is a straight relation between the energy gap and chemical hardness. The higher the energy gap, the more stable the molecule is, ending in a declined reactivity.

Table 5. Chemical hardness (η), and Softness ($1/\eta$) of quinone-based drugs in gas and solution phase.

	Chemical hardness, eV			
Comp.	Gas Phase	MeOH	DMSO	THF
A	0.07544	0.07649	0.07650	0.07632
AH_2	0.10903	0.10978	0.10979	0.10974
B	0.06880	0.06986	0.06987	0.06972
BH_2	0.11446	0.11630	0.11632	0.11612
C	0.05802	0.05696	0.05695	0.05709
CH_2	0.09973	0.06271	0.06268	0.06311
	Softness, 1/eV			
A	13.25556	13.07360	13.07190	13.10273
AH_2	9.17178	9.10913	9.10830	9.11245
B	14.53488	14.31434	14.31229	14.34309
BH_2	8.73668	8.59845	8.59697	8.61178
C	17.23544	17.55618	17.55926	17.51620
CH_2	10.02707	15.94642	15.95405	15.84535

In organic chemistry, an electrophile concept is defined as an electron absorbent. Electrophiles are each of two neutral or positive and have unoccupied orbitals that are transformed into rich middle points in order to absorb electrons. When, two molecules react

as a group, a molecule acts as a nucleophilic system (nucleophilic addition). Whenever the other acts as an electrophilic system (electrophilic addition). The electrophilicity concept was explained for the first time in 1999 by Parr et al [31]. The electrophilicity indices are pertinent to electronic charge. Electrophilicity is a HOMO-LUMO-dependent parameter that changes the structural reactivity. Electrophilicity is adaptable with chemical hardness and chemical potential. This parameter is computed through the following relation [32]:

$$\omega = \frac{\mu^2}{2\eta}. \quad (7)$$

The computational results are indicated in Table 6.

Table 6. Electrophilicity index in quinone-based drugs in gas and solution phase.

Electrophilicity index, eV				
Comp.	Gas Phase	MeOH	DMSO	THF
A	0.25207	0.26294	0.26304	0.26159
AH_2	0.09400	0.09717	0.09722	0.09673
B	0.31047	0.31188	0.31185	0.31185
BH_2	0.08202	0.08140	0.08139	0.08470
C	0.35251	0.35787	0.35793	0.35719
CH_2	0.08954	0.07375	0.07387	0.07254

The dipole moment is a criterion for the non-uniform distribution of charge and expresses the polarity in a molecule [33]. A polar molecule is one that has positive and negative sides. For each polar bond, a polarized vector can be considered, whose direction is toward the more electronegative atom and its length depends on the electronegative difference between the two atoms. The greater the electronegativity difference between two atoms, the larger the dipole moments in the bond and the more polar the bond is (see Table 7).

Table 7. Dipole moment of quinone-based drugs in gas and solution phase.

Dipole moment, D				
Comp.	Gas Phase	MeOH	DMSO	THF
A	0.0038	0.0051	0.0051	0.0050
AH_2	2.8765	3.7544	3.7658	3.6322
B	0.0039	0.0038	0.0038	0.0037
BH_2	2.8925	3.7034	3.7136	3.5928
C	1.4347	1.5552	1.5563	1.5426
CH_2	2.1294	4.6453	4.6563	4.5261

3. CONCLUDING REMARKS

The electrochemical properties of three elected quinones in H_2O, MeOH, DMSO, and THF solvents were theoretically investigated. Oxidation and declined molecule states were ameliorated by implementing the Gaussian 09 software. Therefore, the G° values were calculated in the solution and gas phases. The $\Delta G°_{total}$ values were obtained for each molecule and as a result, the half-wave potential was computed. The $E°_{1/2}$ value of 2, 5-dimethyl-1, and 4-benzoquinone is larger than of the anthraquinone and phenyl-1, 4-benzo quinone. We have demonstrated the antioxidant activity of 2, 5-dimethyl-1, 4-benzoquinone is larger than of the other quinone-based drugs.

The calculations reveal also that the energy gap, electrophilicity, and chemical potential values of the 2, 5-dimethyl-1, 4-benzoquinone are higher than the corresponding values of the anthraquinone and phenyl-1, 4-benzo quinone. Hence, the 2, 5-dimethyl-1, and 4-benzoquinone is more reactive than the other quinones studied. It is suggested that the values of reduction potentials in non-polar and polar solvents calculated at different theoretical levels will surely lead to more accurate results.

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