

# Synthesis and Quantum Chemical Calculations of 2,4-Dioxopentanoic Acid Derivatives-Part II

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**Abstract-** The 2,4-dioxopentanoic acid derivatives (3d-f) were obtained from the reaction of 4-acetyl-5-(1-naphthyl)furan-2,3-dione (1) with various nitrogenous nucleophiles (2d-f). The structures of these newly synthesized compounds (3d-f) were determined from the FT-IR, <sup>1</sup>H and <sup>13</sup>C NMR spectroscopic data and elemental analyses. In addition to experimental analysis, quantum-chemical calculations of derivatives of 2,4-dioxopentanoic acid (3d-f) were carried out by using B3LYP method with basis set of the 6-311G(d,p) in order to find molecular properties. Quantum chemical features such as HOMO, LUMO, HOMO-LUMO energy gap, chemical hardness, chemical softness, electronegativity, chemical potential, dipole moment etc. were calculated and discussed.

**Keywords-** furan-2,3-dione, nitrogenous nucleophiles, 2,4-dioxopentanoic acid, quantum chemical calculations

## I. INTRODUCTION

In early studies, 4-acyl-5-alkyl/aryl-2,3-dihydro-2,3-furandiones were obtained from 1,3-dicarbonyl compounds with oxalyl halides [1-4]. Recently, reactions of cyclic oxalyl compounds were reported to give substituted heterocyclic compounds. In addition, the reactions of substituted 2,3-furandiones have been studied with several semi-/thiosemicarbazones, ureas, thioureas, oximes, various hydrazines, some acetanilides and amides under different conditions [5-14]. Most of these obtained compounds in general are well known for their potential biological activities [15-18].

In view of these important properties, we carried out the reactions of 4-acetyl-5-(1-naphthyl) furan-2,3-dione (1) with 4-nitrophenylhydrazine, 2,4-dinitrophenylhydrazine and 2-nitrophenylamine (2a-c) [19], and 1-naphthylamine, *p*-toluidine and *o*-toluidine (2d-f). The compound (1) was prepared from 1-(2-naphthyl) butane-1,3-dione with oxalylchloride [20]. The 2,4-dioxopentanoic acid derivatives (3d-f) which are  $\alpha$ -ketocarboxylic acids were synthesized from the reactions of the various amines (2d-f) with 4-acetyl-5-(1-naphthyl)furan-2,3-dione (1) (Figure 1).

## II. COMPUTATIONAL DETAILS

In the section of this study, all calculations were carried out using DFT/B3LYP method with 6-311G(d,p) basis sets of Gaussian program [21]. Optimization of synthesized molecules was performed with 6-311G (d,p) basis set. This basis set is known as one of the basis sets that gives more accurate results in terms of the determination of electronic and geometries properties for a wide range of organic compounds. Quantum chemical parameters such as the energy of the highest occupied molecular orbital ( $E_{HOMO}$ ), the energy of the lowest unoccupied molecular orbital ( $E_{LUMO}$ ), HOMO-LUMO energy gap ( $\Delta E$ ), chemical hardness ( $\eta$ ), softness ( $\sigma$ ), electronegativity ( $\chi$ ), chemical potential ( $\mu$ ), dipole moment (DM), global electrophilicity ( $\omega$ ), sum of the total negative charge (TNC) and sum of electronic and zero-point energies (SEZPE) were calculated and discussed [22].

Molecular properties, related to the reactivity and selectivity of the compounds, were estimated following the Koopmans's theorem relating the energy of the HOMO and the LUMO. Electronegativity is estimated using the following equation:

$$\chi \cong -\frac{1}{2}(E_{HOMO} + E_{LUMO}) \quad (1)$$

Chemical hardness ( $\eta$ ) measures the resistance of an atom to a charge transfer [23], it is estimated by using the equation:

$$\eta \cong -\frac{1}{2}(E_{HOMO} - E_{LUMO}) \quad (2)$$

Chemical potential ( $\mu$ ) and electronegativity ( $\chi$ ) can be calculated with the help of the following equations [22].

$$\mu = -\chi \cong \frac{E_{HOMO} + E_{LUMO}}{2} \quad (3)$$

Electron polarizability, called chemical softness ( $\sigma$ ), describes the capacity of an atom or group of atoms to receive electrons [23] and is estimated by using the equation:

$$\sigma = \frac{1}{\eta} \cong -\frac{2}{(E_{HOMO} - E_{LUMO})} \quad (4)$$

The global electrophilicity ( $\omega$ ) is a useful reactivity descriptor that can be used to compare the electron-donating abilities of molecules [24]. Global electrophilicity index is estimated by using the electronegativity and chemical hardness parameters through the equation:

$$\omega = \frac{\chi^2}{2\eta} \quad (5)$$

A high value of electrophilicity describes a good electrophile while a small value of electrophilicity describes a good nucleophile [25].

### III. RESULTS AND DISCUSSION

The cyclocondensation reactions of 1-(2-naphthyl) butane-1,3-dione with oxalyl chloride regioselectively afforded 4-acetyl-5-(1-naphthyl) furan-2,3-dione (1), which exhibits conjugation with double bonds [20].

Herein, we report the synthesis and characterization of 2,4-dioxopentanoic acid derivatives (3d-f) (Figure 1). At room temperature in benzene, mixing of 4-acetyl-5-(1-naphthyl)furan-2,3-dione (1) and corresponding amines (1:1 mol) for about 24 h led to the formation of the novel compounds (3d-f) in approximately 64-74% yield. In moderate conditions, excellent yields of the reactions can be explained by the chemical behaviour of furandiones similar to the compounds (2d-f) towards nucleophiles [6, 19, 26, 27].

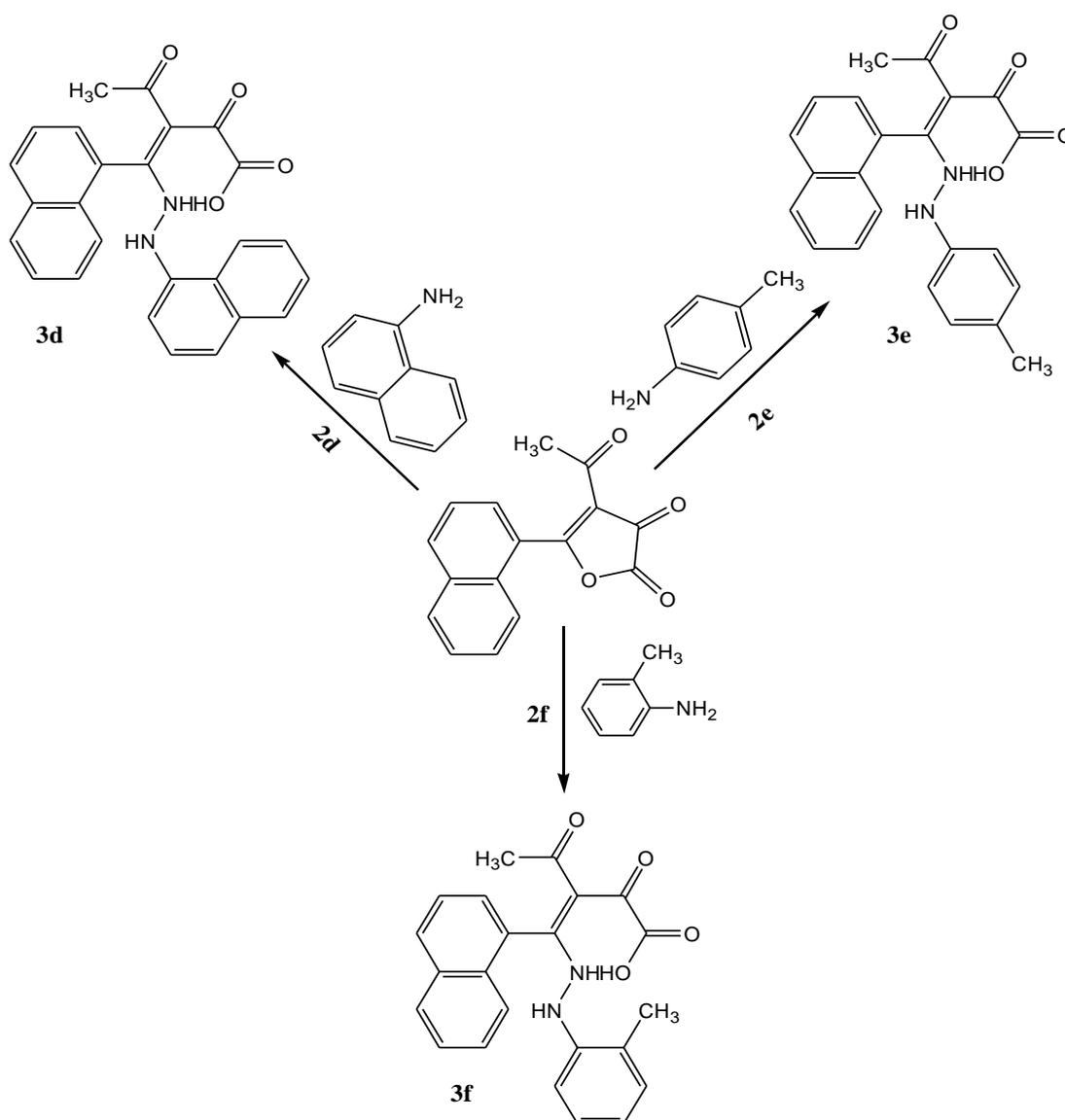


Figure 1. Synthesis of molecules (3d-f).

Addition of the nucleophiles to the furandiones usually starts with nucleophilic attack at one of the C2, C3 and C5 positions of the furan ring system [19, 28-32]. In this reaction, the formation of 2,4-dioxopentanoic acid derivatives (3d-f) may be viewed as occurring *via* a Michael type addition to C5 atom of (1) (Figure 2). The reactions proceeded smoothly at room temperature in benzene for 24 h and afforded the corresponding acid derivatives (3d-f) in yield 64-74%. The new compounds (3d-f) can be used as substrate to obtain the new compounds like the pyrrolidione derivatives.

Structures of synthesized compounds were assigned on the basis of analytical as well as spectroscopic data. Product (3d) was obtained in 64% yield by treating (1) with 1-naphthylamine (2d) and stirring in benzene at room temperature for 24 h. In the IR spectrum of compound (3d), the -OH and -NH absorption bands were found to be at 3500-3200  $\text{cm}^{-1}$ . The absorption bands of C=O groups were seen at 1680, 1580  $\text{cm}^{-1}$ . The  $^1\text{H}$  NMR signals were found to be at  $\delta$ = 11.47 ppm (2H, -OH and -NH) and 8.93-6.70 ppm (m, 14H, aromatic) and 2.55 ppm (s, 3H,  $\text{CH}_3\text{CO}$ ). The  $^{13}\text{C}$  NMR signals were observed at 194.05 ppm ( $\text{CH}_3\text{CO}$ ), 192.35 ppm (C=O), 179.78 ppm (C=O, acide). Finally, the elemental analysis data along with spectroscopic data confirm the structure of 3d. The reaction pathway from 4-acetyl-5-(1-naphthyl) furan-2,3-dione (1) with 1-naphthylamine (2d) to (3Z)-3-[2-Naphthyl(1-naphthylamino)methylene]-2,4-dioxopentanoic acid (3d) is outlined briefly in Figure 1.

Nucleophilic addition of *o*-toluidine (2f) with (1) provided (3Z)-3-[(2-methylphenyl) amino](2-naphthyl)methylene}-2,4-dioxopentanoic acid (3f) in (74%). At the room temperature in benzene, mixing of furan-2,4-dione (1) and *o*-nitroanilin (2f) (1:1 mol) for 24 h. In the IR spectrum of (3f) characteristic absorption bands at about 3600-3100  $\text{cm}^{-1}$  (-OH, -NH) and 1680, 1560  $\text{cm}^{-1}$  (C=O) were observed. The  $^1\text{H}$  NMR signals were at  $\delta$ = 11.11 ppm (-OH and NH), 8.91-6.98 ppm (m, 11H, aromatic), 2.55 ppm (s, 3H,  $\text{CH}_3\text{CO}$ ) and 2.32 ppm (s, 3H,  $\text{CH}_3$ -). The  $^{13}\text{C}$  NMR signals were found to be at 193.10 ( $\text{CH}_3\text{CO}$ ), 192.40 (C=O), 178.88 (C=O, acide), 159.77-113.15 (aromatic C), 28.77 ppm ( $\text{CH}_3\text{CO}$ ) and 17.80 ppm ( $\text{CH}_3\text{C}_6\text{H}_4$ -). Other spectral and analytical data of (3f) are in full agreement with its proposed structure as well.

#### A. Experimental

Solvents were dried by refluxing over the appropriate drying agent and distilled before use. Melting points were determined on an Electrothermal 9200 apparatus and were not corrected. Microanalyses were performed on a Carlo Erba elemental analyzer, model 1108. The IR spectra were recorded on a Shimadzu Model 8400 FT IR spectrophotometer. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker-400 MHz Ultra Shield instrument. The chemical shifts are reported in ppm from tetramethylsilane as an internal standard and are given in  $\delta$  (ppm). All experiments were followed by TLC using DC Alufolien Kieselgel 60 F<sub>254</sub> (Merck) and Camag TLC lamp (254/366 nm).

#### 1) General Procedure for the Preparation of Compounds (3d-f)

To a solution of the compound (1) (2.66 g, 10 mmol) in benzene (50 mL), 1.43 g (10 mmol) 1-naphthylamine (2d) for 3d, 1.07 g (10 mmol) *p*-toluidine (2e) for 3e and 1.07 g (10 mmol) *o*-toluidine (2f) for 3f were added dropwise. After the reaction mixture had been stirred at room temperature for 24 h, and obtained precipitate was filtered and recrystallized from toluene and after allowed to dry on  $\text{P}_2\text{O}_5$ .

#### 2) (3Z)-3-[2-Naphthyl(1-naphthylamino)methylene]-2,4-dioxopentanoic acid (3d)

Yield 0.12 g (64%); m.p.: 130-131 °C; FT-IR  $\nu$  ( $\text{cm}^{-1}$ )= 3500-3200 (-NH, -OH); 1680, 1580 (C=O), 780 (mono-substituted naphthalene);  $^1\text{H}$  NMR (400 MHz, DMSO):  $\delta$ = 11.47 (t, 2H, -NH, -OH), 8.93-6.70 (m, 14H, aromatic), 2.55 (s, 3H,  $\text{CH}_3\text{CO}$ );  $^{13}\text{C}$  NMR (100 MHz, DMSO):  $\delta$ = 194.05 ( $\text{CH}_3\text{CO}$ ), 192.35 (C=O), 179.78 (C=O, acide), 158.27-109.18 ppm (aromatic C), 29.87 ppm ( $\text{CH}_3$ -); Elemental analysis (%): Found (Calc.): C= 76.01 (76.27), H= 4.99, (4.68) and N=3.33 (3.42).

#### 3) (3Z)-3-[(4-Methylphenyl)amino](2-naphthyl)methylene}-2,4-dioxopentanoic acid (3e)

Yield 0.12 g (68%); m.p.: 119-120 °C; FT-IR  $\nu$  ( $\text{cm}^{-1}$ )= 3500-3200 (-NH, -OH); 1680, 1560 (C=O), 750 (mono-substituted  $\text{C}_6\text{H}_4$ -);  $^1\text{H}$  NMR (400 MHz, DMSO):  $\delta$ = 11.53 (t, 2H, -NH, -OH), 8.81-7.14 (m, 11H, aromatic), 2.55 (s, 3H,  $\text{CH}_3\text{CO}$ ), 2.48 ppm (s, 3H,  $\text{CH}_3$ -);  $^{13}\text{C}$  NMR (100 MHz, DMSO):  $\delta$ = 193.15 ( $\text{CH}_3\text{CO}$ ), 192.11 (C=O), 178.98 (C=O, acide), 159.27-121.18 ppm (aromatic C), 28.87 ( $\text{CH}_3\text{CO}$ ), 20.94 ppm ( $\text{CH}_3\text{C}_6\text{H}_4$ -); Elemental analysis (%): Found (Calc.): C= 73.74 (73.98), H= 5.03, (5.13) and N=3.70 (3.75).

#### 4) (3Z)-3-[(2-Methylphenyl)amino](2-naphthyl)methylene}-2,4-dioxopentanoic acid (3f)

Yield 0.12 g (74%); m.p.: 123-124 °C; FT-IR  $\nu$  ( $\text{cm}^{-1}$ )= 3600-3100 (-NH, -OH); 1680, 1560 (C=O), 750 (mono-substituted  $\text{C}_6\text{H}_4$ -);  $^1\text{H}$  NMR (400 MHz, DMSO):  $\delta$ = 11.11 (t, 2H, -NH, -OH), 8.91-6.98 (m, 11H, aromatic), 2.55 (s, 3H,  $\text{CH}_3\text{CO}$ ), 2.32 (s, 3H,  $\text{CH}_3$ -);  $^{13}\text{C}$  NMR (100 MHz, DMSO):  $\delta$ = 193.10 ( $\text{CH}_3\text{CO}$ ), 192.40 (C=O), 178.88 (C=O, acide), 159.77-113.15 ppm (aromatic C), 28.77 ppm ( $\text{CH}_3\text{CO}$ ), 17.80 ppm (s, 3H,  $\text{CH}_3\text{C}_6\text{H}_4$ -); Elemental analysis (%): Found (Calc.): C= 74.16 (73.98), H= 4.96, (5.13) and N=3.80 (3.75).

#### B. Molecular structure

$E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$ ,  $\Delta E$ , DM, MV, TNC,  $\eta$ ,  $\sigma$ ,  $\mu$ ,  $\chi$ ,  $\omega$ , SEZPE were calculated for the 2,4-dioxopentanoic acid derivatives (3d-f) with the B3LYP/6-311G(d,p) method for gas phase and solvent phase, as shown in Figures 3 and 4, and Table 1.

$E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  are associated with electron donating ability and electron accepting ability of a molecule, respectively. Higher  $E_{\text{HOMO}}$  is essential for molecular reaction with nucleophiles while lower  $E_{\text{LUMO}}$  reacts easily with electrophiles [33].  $E_{\text{HOMO}}$  values of 3d-f molecules are found for gas phase -6.06, -6.12, -5.98 eV and for solvent phase -6.10, -6.20, -5.98 eV, respectively (Fig. 3). According to these results, the electron donating trends for study molecules for gas and solvent phase can be written as: 3e>3d>3f. There is no significant change in the  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  values according to the position and number of groups in the ring.

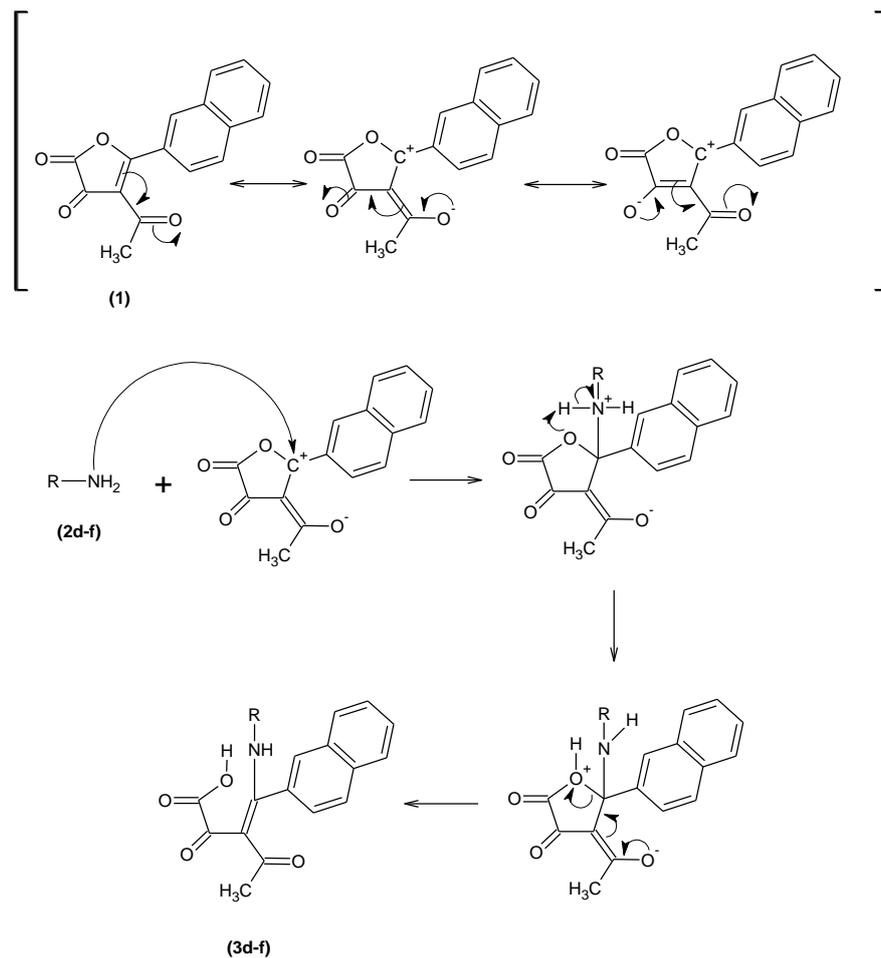


Figure 2. Reaction mechanism of the synthesized compounds (3d-f).

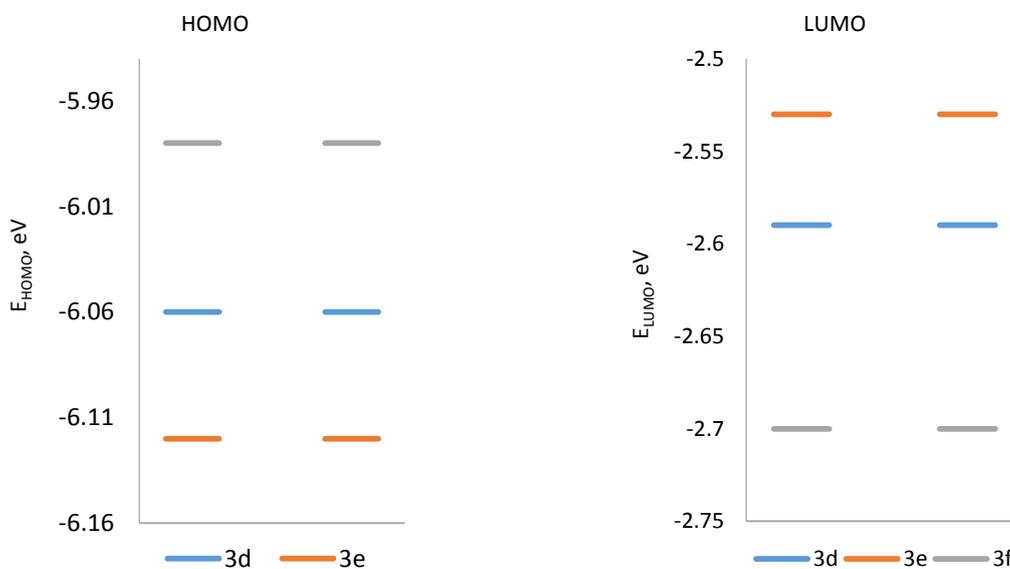


Figure 3. The calculated HOMO and LUMO parameters for neutral molecules for gas and solvent phase using B3LYP/6-311G(d,p) method

HOMO-LUMO energy gap ( $\Delta E$ ), chemical hardness and softness are closely related to chemical properties.  $\Delta E$  value is smaller when the basis set of atomic orbitals are magnified due to the changing of HOMO, usually to a more negative energy and decreasing in energy of LUMO [34]. More stable

molecules have large  $\Delta E$  value and less stable molecules have small  $\Delta E$  value.  $\Delta E$  values for gas phase of 3d, 3e and 3f molecules were found 3.47, 3.59, 3.28 for gas phase and 3.46, 3.58, 3.23 eV for solvent phase, respectively (Table 1).

TABLE I. CALCULATED QUANTUM CHEMICAL PARAMETERS FOR NON-PROTONATED MOLECULES IN GAS AND SOLVENT PHASE

Molecule	Method (B3LYP)	$\Delta E$ , eV	MV, cm <sup>3</sup> /mol	TNC, e	$\mu$ , eV	$\omega$ , D <sup>2</sup> /eV	SEZPE, eV
3d	6-311G(d,p)	3.47	304.249	-3.527	-4.325	9.531	-36948.496
3e	6-311G(d,p)	3.59	259.817	-3.586	-4.325	9.006	-33837.461
3f	6-311G(d,p)	3.28	247.598	-3.660	-4.340	8.461	-33836.067
3d <sup>1</sup>	6-311G(d,p)	3.46	321.343	-3.700	-4.370	16.214	-36948.787
3e <sup>1</sup>	6-311G(d,p)	3.58	275.083	-3.735	-4.410	15.164	-33837.751
3f <sup>1</sup>	6-311G(d,p)	3.23	268.702	-3.829	-4.365	14.723	-33836.348

<sup>1</sup>in the presence of DMSO

3e molecule is found more stable than 3d and 3f molecules due to the fact that a large  $\Delta E$  value is observed. The hardness and softness are widely used in chemistry for explaining stability of compounds. According to Maximum Hardness Principle [34], chemical hardness is a measure of the stability of chemical species. The hardness is just half the energy gap between the  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  (see eq. 2). If a molecule has a large energy gap, it is called hard and other wise is called soft

[35]. Softness is a measure of the polarizability and soft molecules give more easily electrons to an electron acceptor molecule or surface [22]. On the basis of the calculated chemical hardness, softness and energy gap are given in Fig. 4. According to softness values, electron donating trend of studied chemical compounds may be written as: 3f>3d>3e for gas and solvent phase (Fig. 4).

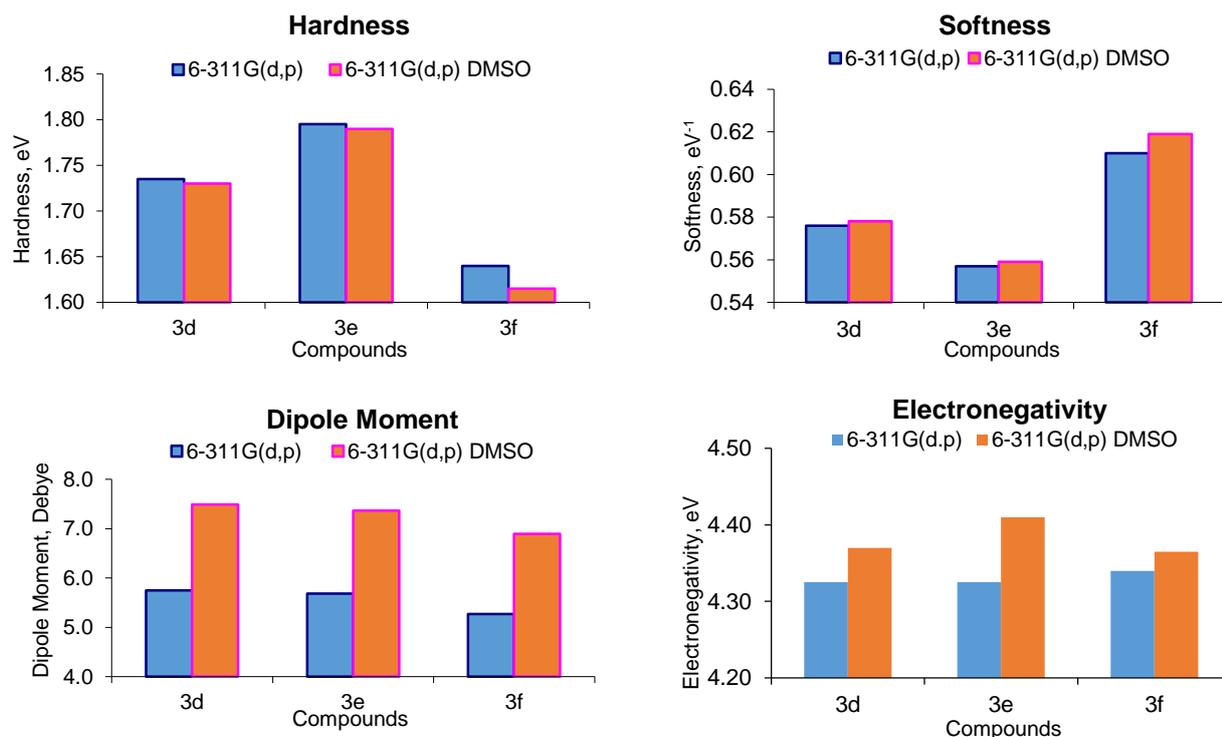


Figure 4. The calculated quantum chemical parameters for the non-protonated for gas and solvent phase compounds using B3LYP/6-311G(d,p) method

The average values of the HOMO and LUMO energies have been defined as the chemical potential ( $\mu$ ). The chemical potential was defined as the first derivative of the total energy with respect to the number of electrons. The negative of the chemical potential was known as the electronegativity ( $\chi$ ) (see eq. 3). Chemical potential, electronegativity and hardness are

descriptors for the predictions about chemical properties of molecules [36]. Electronegativity that represents the power to attract the electrons of chemical species is a useful quantity in the prediction of inhibitive performance of molecules [22]. The electronegativity value of 3f is more than those of 3d and 3e for gas phase (see Fig. 4).

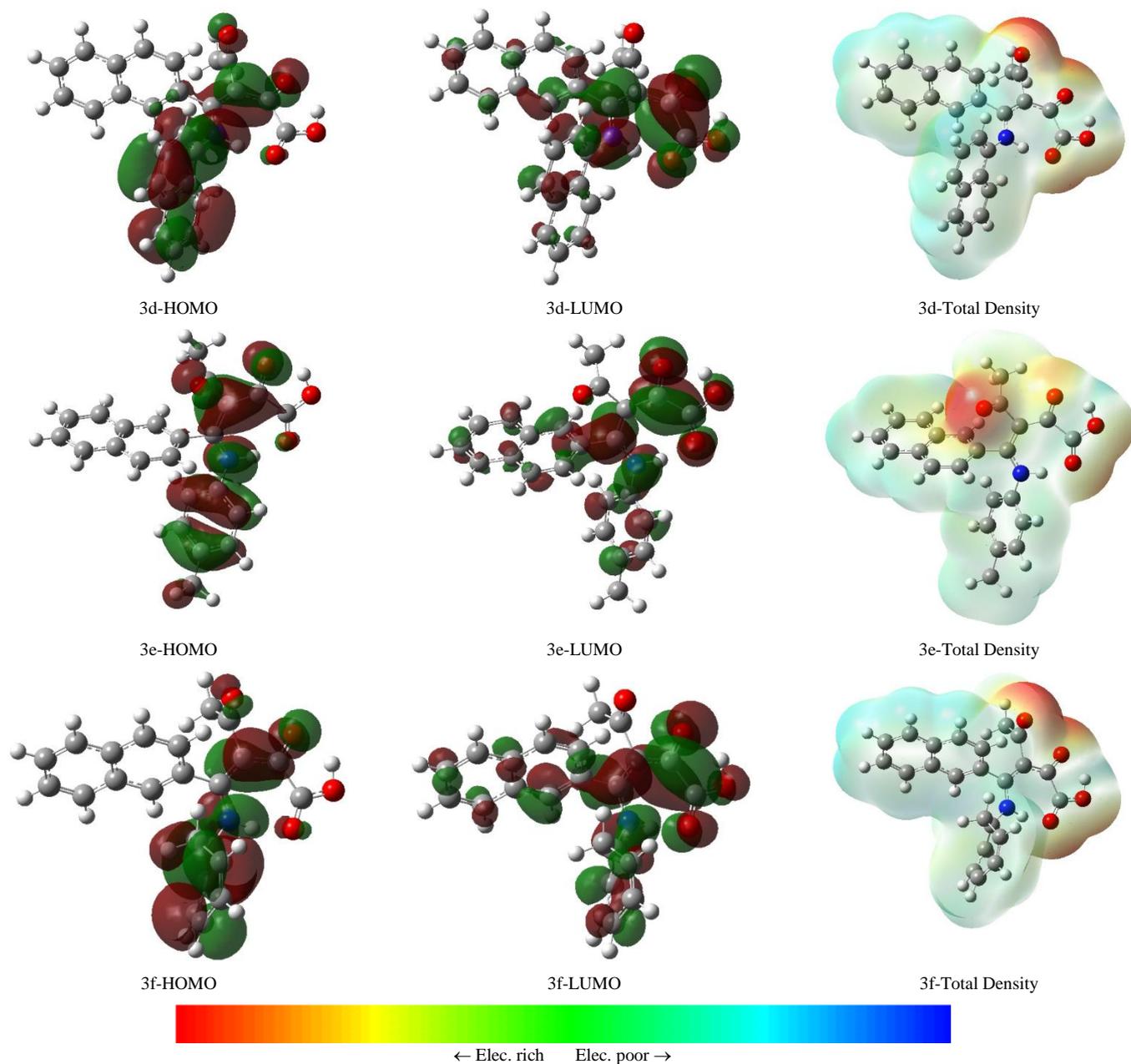


Figure 5. The optimized molecular structures, HOMOs, LUMOs and total density of the non-protonated inhibitor molecules using DFT/B3LYP/6-311G (d,p)

A typical electron density distribution of Total electronic charge (TNC) values calculated with the 6-311G (d,p) basis set. Total electronic charge values are lower in solvent phase than in gas phase (Table 1). As can be seen from Fig. 5, the negative charge densities are concentrated on oxygen atoms for 3d, 3e and 3f molecules.

Sum of electronic and zero-point energies (SEZPE) for 3d molecule containing one naphthyl group is higher than 3e and 3f molecules containing one methyl group (Fig. 5). In Fig. 5 the optimized molecular structures, HOMOs, LUMOs and total electron density are also given in Fig. 5. This figure shows that there is much more electron density in the vicinity of oxygen atoms for all studied molecules.

TABLE II. HOMO AND LUMO POPULATION FOR MOLECULES USING AOMIX METHOD AFTER FROM B3LYP/6-311G METHOD

Mol.	HOMO
3d	- 5.5% 3PZ(C16) - 5.0% 4PZ(C16) + 4.6% 3PZ(N12) + 3.2% 4PZ(N12) - 3.1% 3PX(C44) + 2.5% 3PZ(O18)
3e	+ 10.4% 3PZ(C16) + 9.8% 4PZ(C16) - 7.8% 3PZ(N12) - 5.3% 4PZ(N12) + 4.7% 2PZ(C16) - 4.6% 3PZ(O18)
3f	+ 6.1% 3PX(C41) + 5.6% 4PX(C41) + 5.5% 3PZ(C16) + 5.3% 4PZ(C16) - 4.2% 3PX(C22) - 4.1% 3PZ(N12)
3d <sup>†</sup>	+ 4.1% 3PZ(C16) + 3.8% 4PZ(C16) - 3.4% 3PZ(N12) + 3.2% 3PX(C44) - 2.7% 3PX(C34) + 2.5% 4PX(C44)
3e <sup>†</sup>	+ 9.8% 3PZ(C16) + 9.2% 4PZ(C16) - 7.6% 3PZ(N12) - 5.2% 4PZ(N12) - 4.5% 3PZ(O18) + 4.4% 2PZ(C16)
3f <sup>†</sup>	+ 6.4% 3PX(C41) + 5.9% 4PX(C41) + 4.7% 3PZ(C16) - 4.6% 3PX(C22) + 4.5% 4PZ(C16) - 4.1% 4PX(C22)
Mol.	LUMO
3d	+ 9.0% 3PZ(C15) + 8.4% 4PZ(C15) - 8.0% 3PZ(C11) - 7.0% 3PZ(O18) - 5.7% 4PZ(C11) - 5.1% 4PZ(O18)
3e	- 8.9% 3PZ(C15) + 8.3% 3PZ(C11) - 7.9% 4PZ(C15) + 6.7% 3PZ(O18) + 5.5% 4PZ(C11) + 4.9% 4PZ(O18)
3f	- 8.4% 3PZ(C15) + 8.1% 3PZ(C11) - 7.4% 4PZ(C15) + 6.7% 3PZ(O18) + 5.4% 4PZ(C11) + 4.9% 4PZ(O18)
3d <sup>†</sup>	+ 9.2% 3PZ(C15) + 8.4% 4PZ(C15) - 7.9% 3PZ(C11) - 6.9% 3PZ(O18) - 5.6% 4PZ(C11) - 5.1% 4PZ(O18)
3e <sup>†</sup>	- 9.1% 3PZ(C15) + 8.1% 3PZ(C11) - 8.0% 4PZ(C15) + 6.6% 3PZ(O18) + 5.4% 4PZ(C11) + 4.9% 4PZ(O18)
3f <sup>†</sup>	- 8.6% 3PZ(C15) + 8.0% 3PZ(C11) - 7.5% 4PZ(C15) + 6.6% 3PZ(O18) + 5.4% 4PZ(C11) + 4.9% 4PZ(O18)

<sup>†</sup>in the presence of DMSO

HOMO and LUMO for 3d, 3e, 3f are shown in Table 2. HOMO and LUMO were calculated with AOMix program [37, 38] after optimization of molecules. HOMO orbitals for 3d, 3e, 3c at non-protonated phase consist of - 5.5% 3PZ(C16) - 5.0% 4PZ(C16) + 4.6% 3PZ(N12) + 3.2% 4PZ(N12) - 3.1% 3PX(C44) + 2.5% 3PZ(O18); + 10.4% 3PZ(C16) + 9.8% 4PZ(C16) - 7.8% 3PZ(N12) - 5.3% 4PZ(N12) + 4.7% 2PZ(C16) - 4.6% 3PZ(O18); + 6.1% 3PX(C41) + 5.6% 4PX(C41) + 5.5% 3PZ(C16) + 5.3% 4PZ(C16) - 4.2% 3PX(C22) - 4.1% 3PZ(N12) and their LUMO consist of + 9.0% 3PZ(C15) + 8.4% 4PZ(C15) - 8.0% 3PZ(C11) - 7.0% 3PZ(O18) - 5.7% 4PZ(C11) - 5.1% 4PZ(O18); - 8.9% 3PZ(C15) + 8.3% 3PZ(C11) - 7.9% 4PZ(C15) + 6.7% 3PZ(O18) + 5.5% 4PZ(C11) + 4.9% 4PZ(O18); - 8.4% 3PZ(C15) + 8.1% 3PZ(C11) - 7.4% 4PZ(C15) + 6.7% 3PZ(O18) + 5.4% 4PZ(C11) + 4.9% 4PZ(O18). As seen from Table 2 and given above HOMO orbitals of 3d and 3e molecules for gas and solvent phase consist of mainly C16, N12 and O18 atoms, and HOMO orbitals of 3f molecule for gas and solvent phase consist of mainly C16, C22 and C41 atoms. LUMO orbitals of 3d, 3e and 3f molecules for gas and solvent phase consist of mainly C11, C15 and O18 atoms.

#### IV. CONCLUSIONS

In this study, 2,4-dioxopentanoic acid derivatives (3d-f) were obtained from the reaction of 4-acetyl-5-(1-naphthyl)furan-2,3-dione (1) with various nitrogenous nucleophiles (2d-f). The structures of these newly synthesized compounds (3d-f) were determined from the FT-IR, <sup>1</sup>H and <sup>13</sup>C

NMR spectroscopic data, elemental analyses and in addition to experimental analysis, we calculated and discussed quantum chemical parameters such as the energy of the highest occupied molecular orbital, the energy of the lowest unoccupied molecular orbital, HOMO-LUMO energy gap, chemical hardness, softness, electronegativity, chemical potential, dipole moment, global electrophilicity, sum of the total negative charge (TNC) and sum of electronic and zero-point energies (SEZPE) quantum-mechanical calculations by using B3LYP method with basis set of the 6-311G(d,p) in order to find molecular properties.

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