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Investigation of Theoretical and Experimentical Properties of 2-[3-(n-Propyl)-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl]-Phenoxyacetic Acide

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Abstract: In the present study, 2-[3-(*n*-propyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide was optimized by using B3LYP/6-311+G(d,p) basis set. Firstly, IR data of the compound were calculated in gas phase by using of 6-311+G(d,p) basis set of B3LYP method and are multiplied with appropriate adjustment factors. Theoretical infrared spectrums are formed from the data obtained according to B3LYP method. In the identification of calculated IR data was used the veda4f program. Then, ^{1}H-NMR and ^{13}C-NMR spectral data values were calculated according to the method of GIAO using the program package Gaussian G09W Software. Experimental data were obtained from the literature. Experimental and theoretical values were inserted into the graphic according to equitation of δexp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Furthermore, molecular structure, HOMO and LUMO energy analysis, electronic transitions, total static dipol moment (μ), the mean polarizability (<α>), the anisotropy of the polarizability (Δα), the mean first-order hyperpolarizability (<β>), electronegativity (χ), hardness (η), molecular electrostatic potential maps (MEP), and Mulliken charges of 2-[3-(*n*-propyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide have been investigated by using B3LYP level with the 6-311+G(d,p) basis set.

Keywords: Phenoxyacetic acide, Hyperpolarizability, Theoretical.

Introduction

The development of new heterocyclic organic compounds has received considerable attention due to their potential fluorescence applications as chemosensors (Qin et al., 2015), ionic or biological probes (Mecca et al., 2016; Beytur, 2020) and lighting Technologies (Kido et al., 1995; Sun et al., 2006; Yang et al., 2015; Zhao et al., 2017). The biological activities of the Schiff bases in medicinal chemistry are attributed to the presence of groups in literature (Sztanke et al., 2013; Alkan et al., 2007; Gürsoy-Kol et al., 2010; Aktaş-Yokuş et al., 2017; Bahçeci et al., 2016; Bahçeci et al., 2017; Boy et al., 2021; Koç et al., 2019). Otherwise, Schiff bases have been used as insecticides, bacteriocides, fungicides, pesticides (Azam et al., 2007). In the last year, computational properties of Schiff bases were examined on a computer (Turhan-Irak et. al., 2018; Beytur et al., 2019; Turhan-Irak et. al., 2019; Uğurlu et. al., 2020; Beytur et al., 2021). The optimized molecular structure, vibrational frequencies, spectroscopic parameters, atomic charges and frontier molecule orbitals (HOMO and LUMO) of the 2-[3-(*n*-propyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide have been calculated by using DFT/B3LYP method with 6-311+G(d,p) basis set. All quantum chemical calculations were carried out by using Gaussian 09W (Frisch et al., 2009; Wolinski et. al., 1990) program package and the GaussView molecular visualization program (Frisch et. al., 2003). The molecular structure and vibrational calculations of the molecule were computed by using Becke-3-Lee Yang Parr (B3LYP) (Becke, 1993; Lee et al.,1988) density functional method with 6-311+G(d,p) basis set in ground state. IR absorption frequencies of analyzed molecule were

calculated by two methods. Then, they were compared with experimental data (Çiftçi et al., 2018), which are shown to be accurate. Infrared spectrum was composed by using the data obtained from both methods. The assignments of fundamental vibrational modes of the title molecule were performed on the basis of total energy distribution (TED) analysis by using VEDA 4f program (Jamróz, 2004). Furthermore, molecular structure, HOMO and LUMO energy analysis, electronic transitions, total static dipol moment (μ), the mean polarizability (<α>), the anisotropy of the polarizability (Δα), the mean first-order hyperpolarizability (<β>), electronegativity (χ), hardness (η), molecular electrostatic potential maps (MEP), and Mulliken charges of 2-[3-(*n*-propyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide have been investigated by using B3LYP level with the 6-311+G(d,p) basis set. The titled molecule optimized using *ab* initio Density Functional Theory (DFT/B3LYP), (Becke-3-Lee-Yang-Parr (B3LYP) hybrid density functional), and Hartree-Fock (HF) (Figure 1).

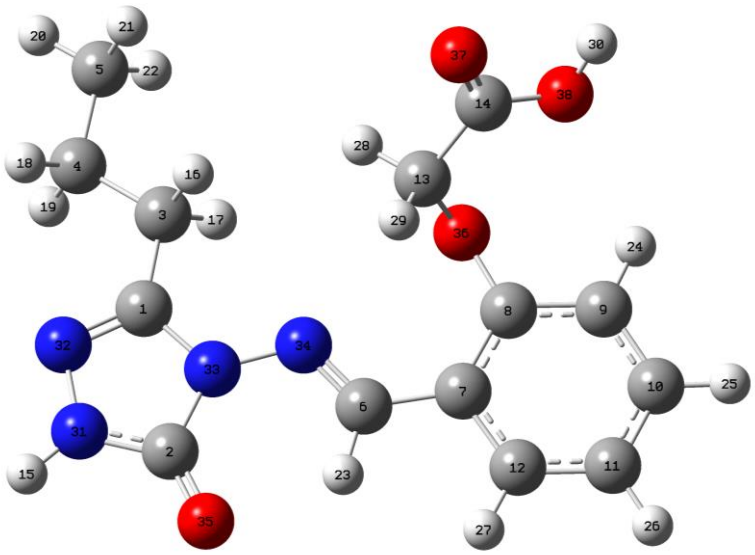


Figure 1. The optimized molecular structure of titled molecule with DFT/HF 6-311+G(d,p) level.

Method

The molecular structure of the title compound in the ground state is computed by performing both the density functional theory (DFT) and Hartree-Fock (HF) (Becke, 1993; Lee, 1998) at 6-311+G(d,p) level. Density functional for all studies reported in this paper have been in the following form

$$E_{XC} = (1-a_0)E_X^{LSDA} + a_0E_X^{HF} + a_X\Delta E_X^{B88} + a_CE_C^{LYP} + (1-a_C)E_C^{VWN}$$

where the energy terms are the Slater exchange, the Hartree-Fock exchange, Becke's exchange functional correction, the gradient corrected correlation functional of Lee, Yang and Parr, and the local correlation functional of Vosko, Wilk and Nusair (Vosko et al., 1980). The theoretical geometric structure of the title compound is given in Figure 1. Molecular geometry is restricted and the optimized geometrical parameters, of the title compound in this study are carried out by using Gaussian 09W program package (Frisch et al., 2009) and the visualization parts were done with GaussView program (Dennington et al., 2009) on personal computer employing 6-311+G(d,p) basis set. Additionally, harmonic vibrational frequencies for the title compound are calculated with these selected methods and then scaled by 0.9516 (Avcı et. al, 2008) and these results were compared with the experimental data (Çiftçi et al., 2018).

Results and Discussion

Vibrational Frequencies

The 2-[3-(*n*-propyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide has 38 atoms and the number of the normal vibrations are 108. The observed and calculated vibrational frequencies, the calculated IR

intensities and assignments of selected vibrational frequencies for title compound are summarized in Table 1 and Figure 2. Experimentally (Çiftçi et al., 2018), the investigated titled compound, as expected the IR spectra data, The S-H stretching vibration at 3425 cm^{-1}, the N-H stretching vibration at 3269 cm^{-1} and two C=O peak at and 1710 cm^{-1} range was observed. In addition, C=N stretching vibration at 1652 and 1592 cm^{-1} and COO stretching vibrations at 1256 cm^{-1} are occurred.

Table 2. The calculated frequencies values of the molecule.

Selected Vibrational Types	Experimental	Scaled DFT
δ $N_{31}N_{32}C_1$, $N_{33}N_{34}C_6$ (23)	758	765
ν $N_{31}C_2$, $N_{33}C_4$ (15), $N_{31}N_{32}$, $N_{33}N_{34}$ (16)	758	770
$O_{38}C_{14}$, $O_{36}C_8$ (18)	809	799
δ $N_{31}N_{32}C_1$, $N_{33}N_{34}C_6$ (13)	957	946
τ $C_{14}C_{13}O_{36}C_8$ (17)	957	980
ν $N_{31}N_{32}$, $N_{33}N_{34}$ (24), ν $N_{31}N_{32}$, $N_{33}N_{34}$ (42), δ $H_{15}N_{31}N_{32}$ (10)	1067	1053
δ $H_{30}O_{38}C_{14}$ (14)	1114	1123
ν $N_{31}C_2$, $N_{33}C_4$ (19), $N_{31}N_{32}$, $N_{33}N_{34}$ (14)	1114	1139
ν $O_{38}C_{14}$, $O_{36}C_8$ (18)	1166	1178
ν $N_{31}C_2$, $N_{33}C_4$ (10)	1166	1180
ν $N_{31}N_{32}$, $N_{33}N_{34}$ (12)	1166	1221
ν $N_{31}N_{32}$, $N_{33}N_{34}$ (10)	1256	1234
δ $H_{30}O_{38}C_{14}$ (14)	1256	1304
δ $H_{15}N_{31}N_{32}$ (66)	1425	1330
ν $N_{32}C_1$, $N_{34}C_6$ (10)	1567	1557
ν $N_{32}C_1$, $N_{34}C_6$ (54)	1592	1565
ν $N_{32}C_1$, $N_{34}C_6$ (65)	1653	1578
ν $O_{35}C_2$ (73)	1710	1697
ν $O_{37}C_{14}$ (87)	1710	1721
ν C_3H_{16}, $C_{13}H_{17}$, C_4H_{18}, C_4H_{19}, C_5H_{20}, C_5H_{21}, C_5H_{22} (71)	2870	2897
ν C_9H_{24}, $C_{10}H_{25}$, $C_{11}H_{26}$, $C_{12}H_{27}$ (10)	2920	2989
ν C_9H_{24}, $C_{10}H_{25}$, $C_{11}H_{26}$, $C_{12}H_{27}$ (100)	2965	2995
ν C_9H_{24}, $C_{10}H_{25}$, $C_{11}H_{26}$, $C_{12}H_{27}$ (84)	3012	3023
ν C_9H_{24}, $C_{10}H_{25}$, $C_{11}H_{26}$, $C_{12}H_{27}$ (98)	3025	3039
ν C_9H_{24}, $C_{10}H_{25}$, $C_{11}H_{26}$, $C_{12}H_{27}$ (94)	3042	3057
ν $N_{31}H_{15}$ (100)	3269	3498
ν $O_{38}H_{30}$ (100)	3425	3567

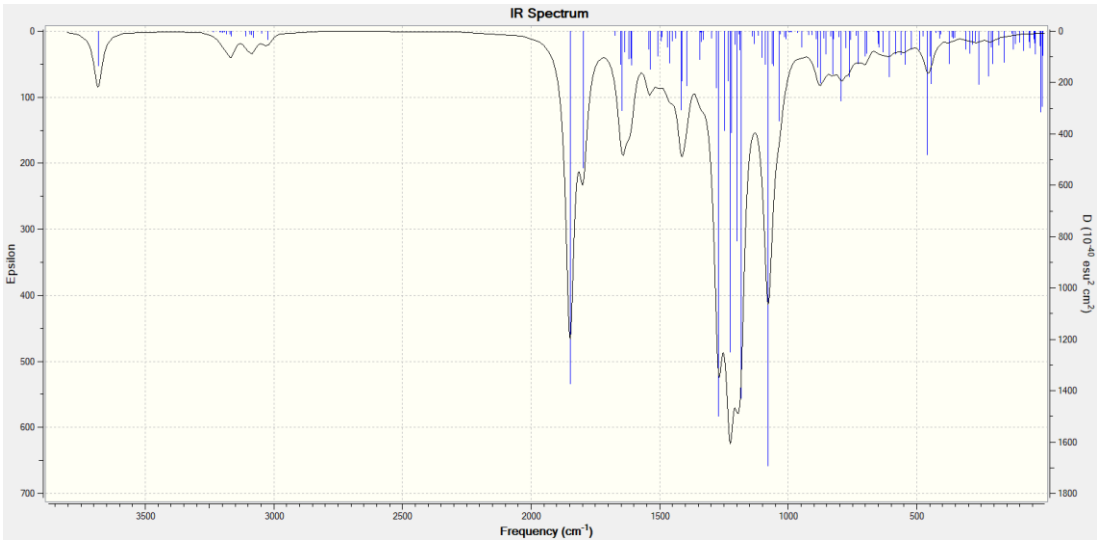


Figure 2. IR spectra simulated with DFT/B3LYP/6-311+G(d,p) level of the titled molecule

NMR Spectral Analysis

In nuclear magnetic resonance (NMR) spectroscopy, the isotropic chemical shift analysis allows us to identify relative ionic species and to calculate reliable magnetic properties which provide the accurate predictions of

molecular geometries (Rani et al., 2010; Subramanian et. al., 2010; Wade, 2006). In this framework, the optimized molecular geometry of the molecule was obtained by using B3LYP method with 6-311+G(d,p) basis level in DMSO solvent. By considering the optimized molecular geometry of the title compound the ^{1}H and ^{13}C NMR chemical shift values were calculated at the same level by using Gauge-Independent Atomic Orbital (GIAO) method. Theoretical and experimental (Çiftçi et al., 2016) values were plotted according to δ exp=a. δ calc.+ b, Eq. a and b constants regression coefficients with a standard error values were found using the SigmaPlot program.

The (R^2) values (DFT) for ^{1}H NMR (DMSO) and ^{13}C NMR (DMSO) chemical shifts in different solvents has been found as 0.9962/07837 for the titled compound (Table 2 and Figure 3). In our study, the ^{1}H-NMR spectrum of compound was observed belong to H15 proton peak at 11.85 ppm because acidic show feature (Yüksek, 1992). H23 proton was observed at 10.05 ppm. Therotically, in DMSO solvents these values for the mentioned proton atoms were found as 7.73 and 10.43 ppm, respectively (B3LYP).

Table 2. The calculated and experimental ^{1}H and ^{13}C NMR isotropic chemical shifts of the titled molecule.

No	Experim.	B3LYP/ DMSO	Diff. /DMSO	No	Experim.	B3LYP/ DMSO	Diff. /DMSO
1C	147,47	155,95	-8,48	15H	11,85	7,73	4,12
2C	151,78	155,87	-4,09	16H	2,65	2,70	-0,05
3C	27,24	30,89	-3,65	17H	2,65	2,81	-0,16
4C	19,41	20,06	-0,65	18H	1,69	1,77	-0,08
5C	13,96	13,99	-0,03	19H	1,69	1,54	0,15
6C	149,60	157,84	-8,24	20H	0,96	1,24	-0,28
7C	122,41	132,00	-9,59	21H	0,96	0,98	-0,02
8C	157,60	165,07	-7,47	22H	0,96	0,99	-0,03
9C	121,80	131,15	-9,35	23H	10,05	10,48	-0,43
10C	126,07	137,25	-11,18	24H	7,92	7,91	0,01
11C	113,29	130,22	-16,93	25H	7,48	7,66	-0,18
12C	133,26	141,65	-8,39	26H	7,09	7,52	-0,43
13C	65,28	73,74	-8,46	27H	7,04	7,74	-0,70
14C	170,40	179,74	-9,34	28H	4,86	5,02	-0,16
				29H	4,86	4,42	0,44
				30H	13,15	6,73	6,42

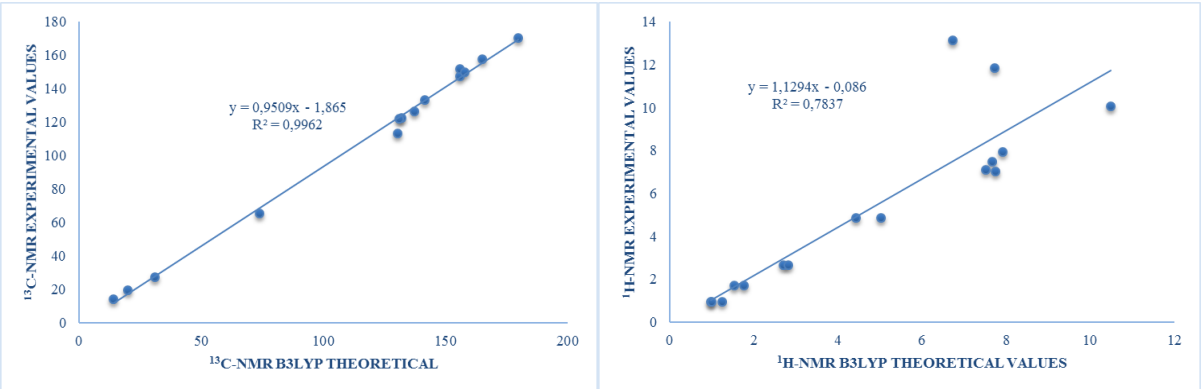
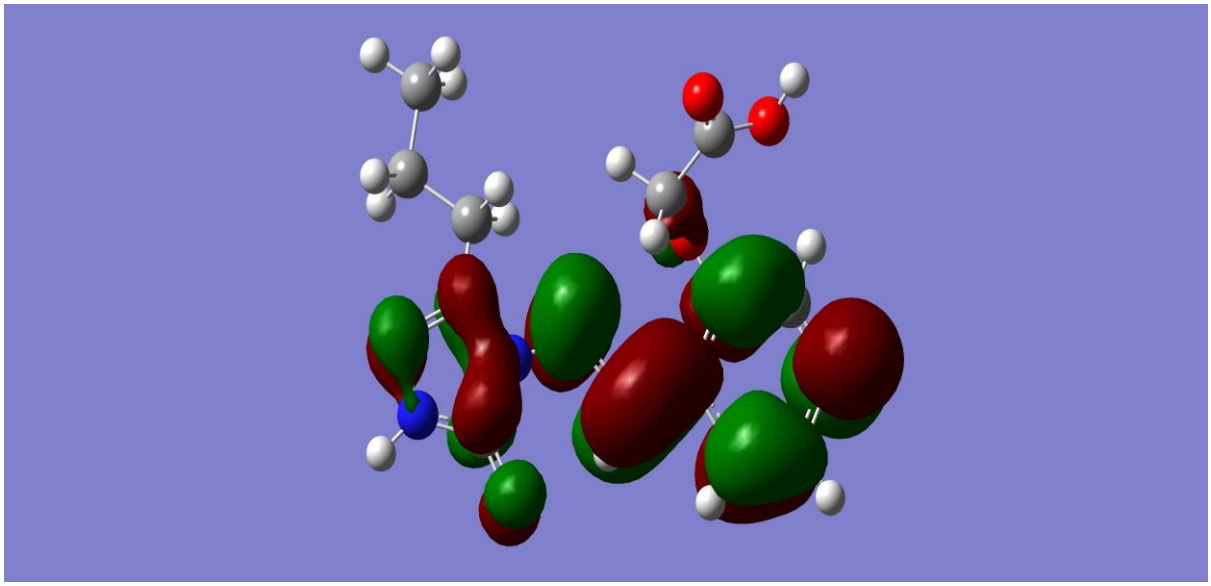


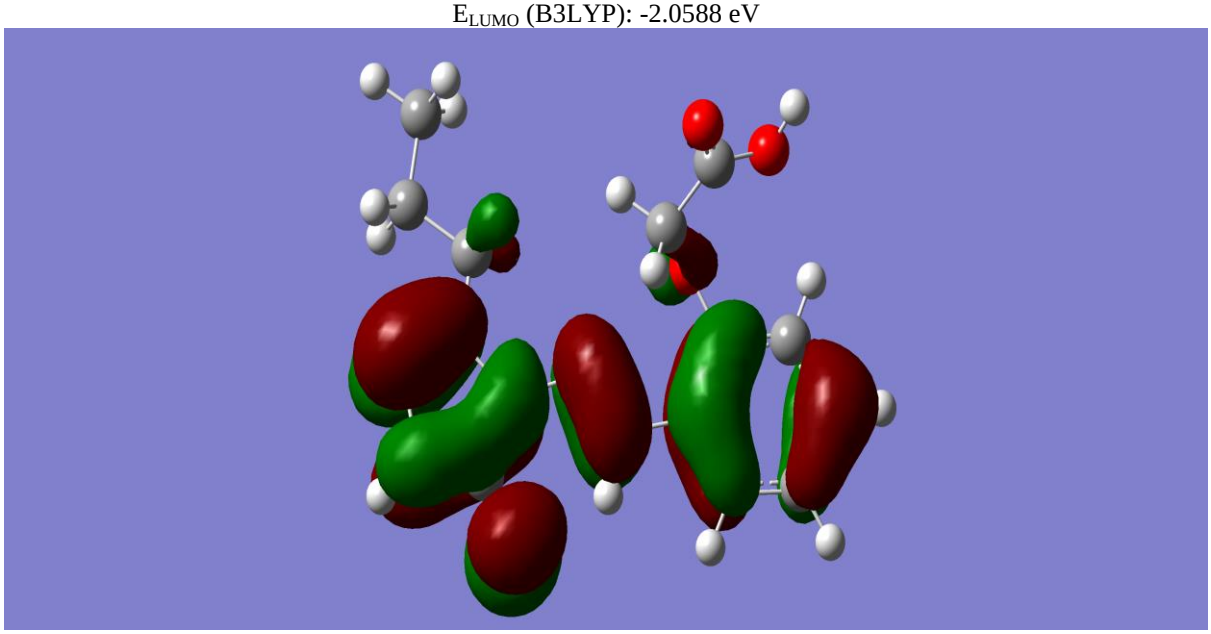
Figure 3. The correlation graphics for ^{13}C-NMR (DMSO) and ^{1}H-NMR (DMSO) chemical shifts of the titled molecule

Electronic and Nonlinear Optic Properties

Identifiers derived from the electronic structure of the 2-[3-(n-propyl)-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide, which are linked to the electronic structure, are called electronic structure identifiers. Some of them are, the Energy of the Highest Occupied Molecular Orbital, Energy of the Lowest Unoccupied Molecular Orbital (Figure 4), molecular hardness, chemical softness, electronegativity, chemical potential, electrophilicity index, nucleophilicity index and dipole moment (Table 3).



E_{LUMO} (B3LYP): -2.0588 eV



E_{HOMO} (B3LYP): -6.4280 eV

Figure 4. The calculated HOMO-LUMO energies of the molecule according to DFT/B3LYP/6-311+G(d,p level

Table 3. Electronic properties of the molecule

	DFT (eV)
Ionization Potential	6.4280
Electron Affinity	2.0588
Electronegativity	4.2434
electrophilic index	0.0531
Nucleophilic index	-0.6814
molecular softness	2.1846
Chemical Hardness	4.3692

The materials having nonlinear activity possess a nonlinear response to the electric fields associated with the light of a laser beam. It is well known that the higher values of dipole moment, polarizability, and hyperpolarizability are important for more active NLO properties. In this study dipole moment, polarizability and first hyperpolarizability of conformer ct of the titled molecule were investigated by using B3LYP method at 6-311+G(2d,p) basis set. The following formulas are used for calculating the magnitude of total static dipole moment (μ), polarizability (α) and first hyperpolarizability (β):

$$\mu = \left(\mu_x^2 + \mu_y^2 + \mu_z^2\right)^{\frac{1}{2}}$$

$$\alpha = \frac{1}{3}\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right)$$

$$\beta = \sqrt{\left(\beta_{xxx} + \beta_{yyy} + \beta_{zzz}\right)^2 + \left(\beta_{yyy} + \beta_{xxy} + \beta_{yzz}\right)^2 + \left(\beta_{zzz} + \beta_{xxz} + \beta_{yyz}\right)^2}$$

Where, the total static dipole moment (μ), linear polarizability (α) and the first hyperpolarizability (β) using the *x*, y, *z* components are defined. The energy gap ΔE_g, dipole moment (μ), linear polarizability (α) and the first hyperpolarizability (β) values of conformer ct of the titled molecule are investigated as a function of the two torsional angle using B3LYP/6-311+G(d,p) level of theory. The calculated results showed that behavior of dipole moment (μ), linear polarizability (α) and the first hyperpolarizability (β) values of conformer ct of the titled molecule as a function of dihedral angles have the same tendency. It means that these values are symmetric with the orthogonal conformation (90º) of the molecules (Govindarajan et al., 2012) (Table 4).

Table 4. Calculated polarization and hyperpolarizability values of the molecule (B3LYP/6-311+G(d,p)

	B3LYP
α_{xx}	44.314a.u.
α_{yy}	33.651 a.u.
α_{zz}	20.016 a.u.
α	32.660×10^{-24} esu
Δα	21.095×10^{-24} esu
β_x	6189.793 a.u.
β_y	346.476 a.u.
β_z	-591.377 a.u.
β_{xxx}	4874.76 a.u.
β_{xxy}	647.84 a.u.
β_{xyy}	667.19 a.u.
β_{yyy}	1006.03 a.u.
β_{xxz}	-515.19 a.u.
B_{xyz}	-144.36 a.u.
B_{yyz}	-321.22 a.u.
β_{xzz}	-29.81 a.u.
β_{yzz}	-240.35 a.u.
B_{zzz}	230.74 a.u.
β	6.23×10^{-30} esu

Dipole Moment and Total Energy

The energetic behavior of title molecule was investigated in vacum. Dipol moments and total energy values of title molecule were calculated by using B3LYP/6-311+G(d,p) level. The calculated dipole moments and total energy values are given in Table 5.

Table 5. The calculated dipole moment values of the molecule

Dipole Moment	B3LYP (a.u.)
μ_x	1.6261
μ_y	0.7175
μ_z	-1.1089
μ_{Toplam}	2.0949

Mulliken's Atomic Charges

The Mulliken atomic charges at the B3LYP/6-311+G(d,p) level of 2-[3-(n-propyl)-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide in gas phase are given in Table 6 (Mulliken, 1955).

Table 6. Mulliken atomic charges of the molecule

Atom	DFT	Atom	DFT	Atom	DFT	Atom	DFT
1C	-0.2816	11C	-0.2652	21H	0.1336	30H	0.2797
2C	0.4787	12C	-0.4546	22H	0.1348	31N	-0.2122
3C	0.3511	13C	-0.2777	23H	0.1766	32N	-0.1559
4C	-0.4702	14C	0.0532	24H	0.1485	33N	-0.1194
5C	-0.5218	15H	0.3325	25H	0.1343	34N	-0.0263
6C	0.0859	16H	0.1623	26H	0.1304	35O	-0.3797
7C	1.0299	17H	0.1851	27H	0.1376	36O	0.0094
8C	-0.6189	18H	0.1588	28H	0.1913	37O	-0.2885
9C	-0.2796	19H	0.1559	29H	0.1877	38O	-0.2199
10C	-0.2313	20H	0.1451				

Conclusion

In this paper, the structure of the titled compound is characterized by using FT-IR, ^{1}H and ^{13}C NMR spectroscopic methods. The molecular structures, vibrational frequencies, ^{1}H and ^{13}C NMR chemicals shifts, UV–vis spectroscopies, HOMO and LUMO analyses and atomic charges of 2-[3-(n-propyl)-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide synthesized for the first time have been calculated by using DFT/B3LYP method. By considering the results of experimental works it can be easily stated that the ^{1}H and ^{13}C NMR chemical shifts, and vibrational frequencies spectroscopic parameters obtained theoretically are in a very good agreement with the experimental data. Also, the electronic structure of titled compound are determined electronic structure identifiers such as the Energy of the Highest Occupied Molecular Orbital, Energy of the Lowest Unoccupied Molecular Orbital, molecular hardness, chemical softness, electronegativity, chemical potential, electrophilicity index, nucleophilicity index and dipole moment. Finally, in this study, The nonlinear optical properties of the compound were calculated theoretically. It was found that the molecule concerned had a higher hyperpolarizability value than urine ($0.77x10^{-30}$esu).

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

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