ICBAST 2022: International Conference on Basic Sciences and Technology

Density Functional Theory and *Ab Initio* Hartree-Fock Computational Study of 2-[1-Acetyl-3-Methyl-4,5-Dihydro-1*H*-1,2,4-Triazol-5-One-4-Yl]-Phenoxyacetic Acide

Murat BEYTUR
Kafkas University

Haydar YUKSEK
Kafkas University

Abstract: In the present theoretical study, the 2-[1-acetyl-3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide was optimized by B3PW91 and HF methods 6-311+G (d.p) basis set using the Gaussian G09W program. The molecular structure, HOMO and LUMO energy analysis, electronic transitions, total static dipole moment, the mean polarizability, the anisotropy of the polarizability, the mean first-order hyperpolarizability, electronegativity, chemical hardness, molecular electrostatic potential maps (MEP) and Mulliken charges of 2-[1-acetyl-3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide molecule have been investigated by using B3PW91 and HF methods with the 6-311+G (d, p) basis set. The calculated IR data of titled compound were calculated in gas phase by using of 6311+G (d, p) basis sets of B3PW91 and HF methods and are multiplied with appropriate adjustment factors. Theoretical infrared spectrums are formed from the data obtained according to B3PW91 method. In the identification of calculated IR data was used the veda4f program. ^{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 δ exp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. In addition, *in vitro* antioxidant properties of this compound was investigated.

Keywords: Gaussian, Schiff base, B3PW91, HF, Spectroscopic, MEP.

Introduction

Heterocyclic compounds containing atoms such as Nitrogen, Oxygen and sulfur exhibit a variety of chemical, theoretical and biological applications as a result of their structural diversity (Bahçeci et al., 2016; Bahçeci et al., 2017; Çiftçi et al., 2018; Beytur et al., 2019a; Beytur et al., 2019b; Irak & Beytur, 2019; Gürsoy Kol et al.,2020; Koç et al., 2020; Kotan et al., 2020; Beytur, 2020; Sertçelik et al., 2020; Uğurlu & Beytur, 2020; Beytur & Avinca, 2021; Boy et al, 2021). Computational chemistry is the atomic and molecular modeling of chemistry in computer environment. Scientists need to calculate very cheaply and quickly by computers without the need for physical experiments that can be achieved by working in laboratories. Physicists and chemists have preliminary information about the structure of drugs before synthesis by making calculations on the computer and enable them to determine the desired properties in the drug (Uğurlu et al., 2007; Uğurlu, 2019; Uğurlu, 2020; Uğurlu & Beytur, 2020).

The molecular structure, HOMO and LUMO energy analysis, electronic transitions, total static dipole moment, the mean polarizability, the anisotropy of the polarizability, the mean first-order hyperpolarizability, electronegativity, chemical hardness, molecular electrostatic potential maps (MEP) and Mulliken charges 2-[1-acetyl-3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide molecule have been calculated

by using B3PW91 (Figure 1) and HF methods with the 6-311+G (d, p) basis set. The calculated IR data of titled compound were calculated in gas phase. ^{1}H-NMR and ^{13}C-NMR spectral data values were calculated according to the method of GIAO. All quantum chemical calculations were carried out by using Gaussian 09W (Wolinski et al., 1990; Frisch et al., 2009) program package and the GaussView molecular visualization program (Frisch et al., 2003). 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 (Jamroz, 2004).
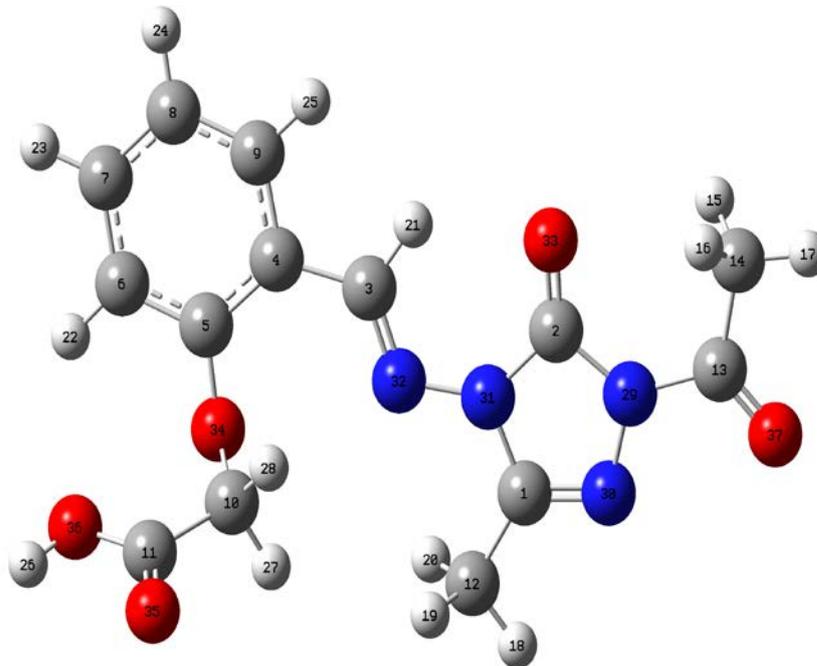
Figure 1. The optimized molecular structure of titled molecule with B3PW91 6-311+G(d,p) level.

Method

All quantum chemical calculations were carried out by using Gaussian 09W (Wolinski et al., 1990; Frisch et al., 2009) program package and the GaussView molecular visualization program (Frisch et al., 2003). The The molecular structure, HOMO and LUMO energy analysis, electronic transitions, total static dipole moment, the mean polarizability, the anisotropy of the polarizability, the mean first-order hyperpolarizability, electronegativity, chemical hardness, molecular electrostatic potential maps (MEP) and Mulliken charges 2-[1-acetyl-3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide molecule have been calculated by using B3PW91 and HF methods with the 6-311+G(d,p) basis set. The vibrational wavenumbers, ^{1}H and ^{13}C NMR chemical shifts of titled compound in ground state have been calculated by using B3PW91 and HF methods (Lee et al., 1988; Hurst, et al., 1988; Becke, 1993). Additionally, B3PW91 and HF methods were also used in the calculations of dipole moment, polarizability and the first-order hyperpolarizability of the titled compound.

Results and Discussion

Investigation of Electronic Properties

In these chemical reactions, HOMO energy is defined as electron donor tendency (π-donor), and LUMO energy is defined as electron acceptor tendency (π-acceptor) (Figure 2) (Fukui, 1982). The electronic properties were calculated by applying the 6-311G+(d,p) diffused and polarized basis set and the B3LYP and HF methods to the molecule. From the calculated HOMO-LUMO energies, electronic parameters such as I; Ionization potential, A; electron affinity, η; molecular hardness, S; molecular softness and χ; electronegativity, total energies, dipole moment values were determined (Table 1).

1a

1b

E$_{LUMO}$: -2.303 eV

ΔE =**4.476 eV**

E$_{HOMO}$: -6.778 eV

E$_{LUMO}$: -1.459 eV

ΔE =**7.737 eV**

E$_{HOMO}$: 9.196 eV
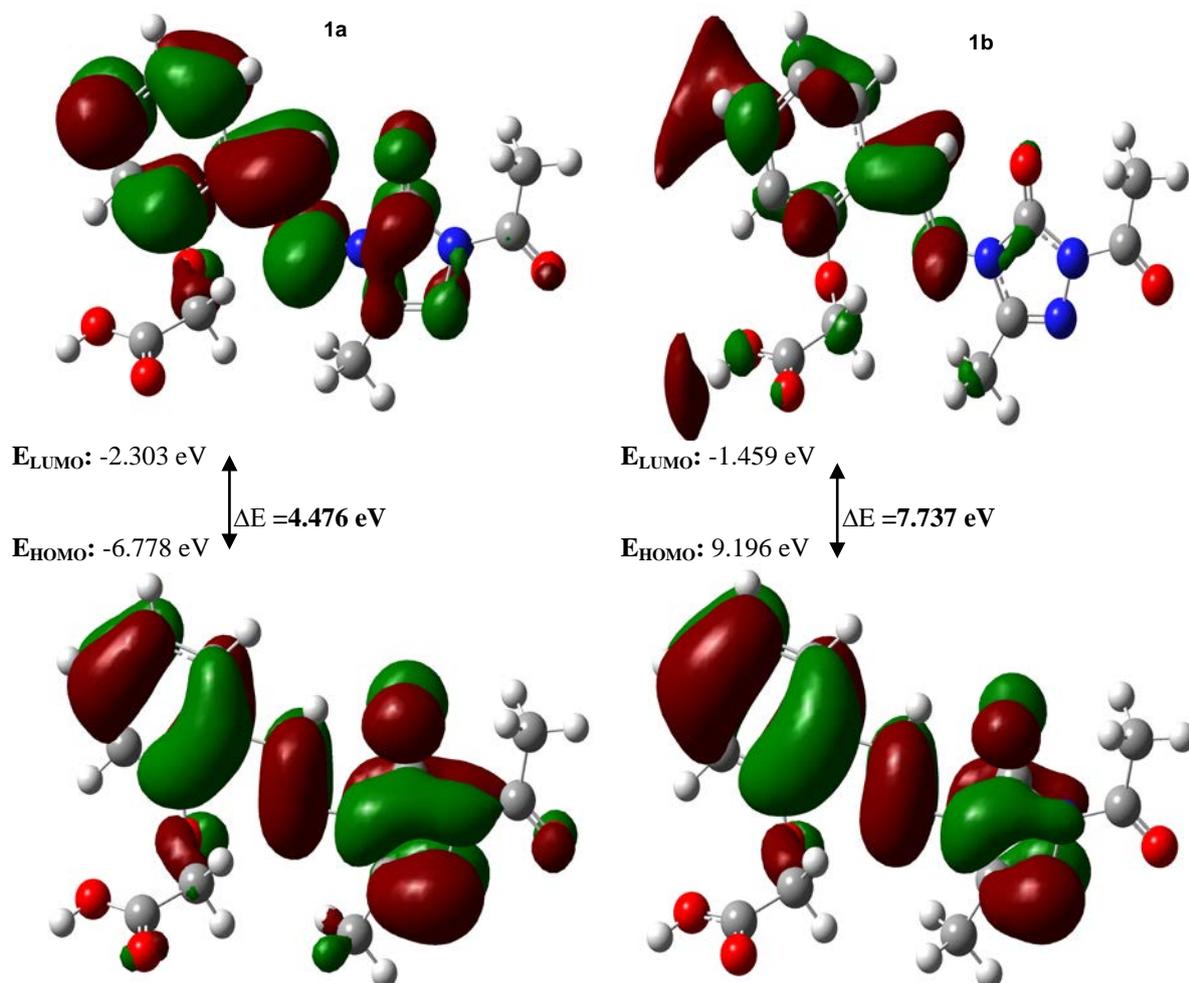
Figure 2. Calculated HOMO-LUMO shapes of the molecula by B3PW91(a) and HF (b) methods 6-311+G (d.p) basis set

Table 1**.** Electronic properties of the molecule calculated according to B3PW91 and HF methods 6-311+G (d.p) basis set

Electronic Features	B3PW91 (eV)	HF (eV)
I; Ionization Potential	6.778	9.196
A; Electron Affinity	2.303	1.459
η; Molecular Hardness	2.238	3.868
S; Molecular Softness	1.119	1.934
χ; Electronegativity	4.541	5.328
ω: electrophilic index	4.606	3.669
ε: Nucleophilic index	-0 373	-0.737
ΔE; Energy Gap	4.476	7.737

Molecular Electrostatic Potential (MEP)

MEP is related to electron density and plays an important role in identifying sites for electrophilic and nucleophilic reactions (Scrocco & Tomasi, 1973; Luque et al, 2000). Different values of electrostatic potential at the Molecular Surface are indicated by different colors. Potential increases are respectively red < orange < yellow < green < blue. The blue areas represent the strongest attraction and the red the strongest repulsion. Negative (red and yellow) regions of MEB are expressed by electrophilic reactivity and positive (blue) regions by nucleophilic reactivity (Figure 3). From the MEP it can be seen that the negative charge covers the heteroatoms and the positive region is above the remaining groups (Kobinyi et al., 1998; Moro et al., 2005).
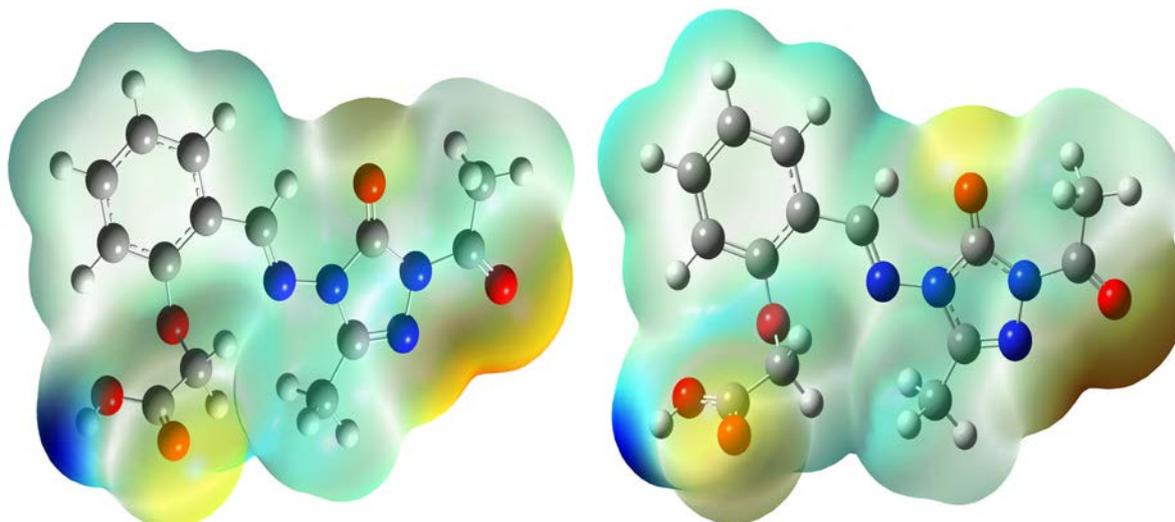
Figure 3. Molecular electrostatic potential of the molecula by B3PW91 and HF methods 6-311+G (d.p) basis set

Mulliken Charges

Mulliken atomic charge calculation is an important atomic charge in the application of quantum chemical calculation to the molecular system (Mulliken, 1995; Ramalingan et al., 2010). Furthermore, Mulliken determines how charges directly affect the vibrational properties of the molecule under study and measures how the electronic structure changes under atomic displacement. Mulliken charges were calculated for the titled molecule and the results are presented in Table 2. Mulliken charge atoms attached to hydrogen atoms were determined to be negative.

Table 2. Mulliken atomic charges of the molecule by B3PW91 and HF methods 6-311+G (d.p) basis set

Atoms	B3PW91	HF	Atoms	B3PW91	HF
1C	0.225555	0.361715	19H	0.161393	0.155796
2C	0.238735	0.422223	20H	0.178250	0.174566
3C	0.151893	0.197584	21H	0.172364	0.191497
4C	0.972007	1.403917	22H	0.150436	0.167786
5C	-0.860028	-0.916166	23H	0.136472	0.144188
6C	-0.174435	-0.370664	24H	0.131989	0.139187
7C	-0.221834	-0.269179	25H	0.135978	0.142539
8C	-0.317004	-0.398733	26H	0.281779	0.311750
9C	-0.253715	-0.389073	27H	0.188723	0.181477
10C	-0.263888	-0.267690	28H	0.187378	0.179172
11C	0.061240	0.228059	29N	0.038007	0.050025
12C	-0.453014	-0.472563	30N	0.032874	0.022434
13C	0.320455	0.525582	31N	-0.282128	-0.448919
14C	-0.423240	-0.469778	32N	-0.192886	-0.253582
15H	0.172502	0.165157	33O	-0.334851	-0.467869
16H	0.173751	0.168737	34O	0.005457	-0.005708
17H	0.176191	0.174242	35O	-0.288277	-0.378062
18H	0.183341	0.184509	36O	-0.220242	-0.314763
			37O	-0.191230	-0.269391

Vibrational frequencies

Vibration frequencies and vibration spectra to determine the functional groups in the structure of 3-ethyl-4-(3-acetoxy-4-methoxy-benzylideneamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one calculated. The harmonic vibrational frequencies were calculated by using B3PW91 and HF methods with the 6-311+G (d,p) basis set (Table 3). The calculated vibration spectra are obtained from the optimized structure, which shows that the potential energy is located at the lowest energy surface. However, the calculated DFT 'non-scale' harmonic

vibration frequencies are known to overestimate the experimental values due to insufficient fundamental clusters, mismatch and lack of electron correlation.

Theoretically found excess values can be adjusted by applying the scaling factors B3PW91 (0.9805) and HF (0.9613) (Foresman, 1996; Tamer et al., 2015). The titled compound has 37 atoms and the number of the normal vibrations are 105. The observed and calculated vibrational frequencies, the calculated IR intensities and assignments of selected vibrational frequencies for title compound are summarized in Table 3 and simulated IR spectra were given in Figure 4.

Table 3. The calculated frequencies values and vibration types of the molecule.

Vibration Types	Experim.	Scaled DFT	Scaled HF
$C_9C_4C_3N_{32}$, $N_{32}C_1C_2N_{31}$, $C_3N_{32}N_{31}C_2$ (76)		10	7
$C_{10}O_{34}C_5C_6$, $O_{36}C_{11}C_{10}O_{34}$ (64)		27	23
$N_{32}C_3C_2N_{30}$, $C_4C_3N_{32}N_{31}$, $O_{36}C_{11}C_{10}O_{34}$ (61)		33	35
$C_{10}O_{34}C_5C_6$, $C_{11}C_{10}O_{34}C_5$ (72)		37	38
$C_3N_{32}N_{31},C_9C_4C_3$, $C_4C_3N_{32},C_{10}O_{34}C_5C_6$ (66)		52	48
$C_{11}C_{10}O_{34}C_5$ (56)		59	58
$C_5C_6C_7C_8,C_2N_{29}N_{30}C_3,C_{13}C_2N_{30}N_{29}$ (36)		72	69
$C_3N_{32}N_{31}C,C_{10}O_{34}C_5C_6$ (26)		82	89
$C_9C_4C_3$ (14)		122	122
$C_{13}C_2N_{30}N_{29},C_3N_{32}N_{31}C_2$ (39)		127	128
$H_{15}C_{14}C_{13}N_{29}$, $C_{12}N_{31}N_{30}C_1$ (46)		147	155
$H_{15}C_{14}C_{13}N_{29}$, $C_{12}N_{31}N_{30}C_1$ (32)		151	162
$H_{18}C_{12}C_1N_{31},H_{20}C_{12}C_1N_{31}$ (77)		173	174
$C_3N_{32}N_{32}N_{31}C_1,C_9C_4C_3N_{32},C_2N_{29}N_{30}C_1$, $C_{12}C_{13}H_{30}C_{13}$ (79)		175	183
$C_5C_6C_7C_8C_9$, $C_{12}C_1N_{30}$ (23)		194	197
$C_{12}C_1N_{30}$, $N_{32}C_1C_2N_{31}$ (21)		211	212
$C_4C_3,C_3N_{32}N_31$(22)		227	234
$O_{34}C_5C_6,C_{11}C_{10}O_{34}$ (39)		240	250
$O_{34}C_5C_6,C_{10}O_{34}C_5,C_5C_6C_7C_8$ (40)		292	305
$C_{12}CN_{30}$ (24)		333	343
$C_2N_{31}N_{30}C_1$ (57)		351	368
$C_5C_6C_7C_8,C_4C_3N_{32}N_{32}N_{31}$(45)		359	379
$C_{12}C_1N_{30},O_{33}C_2N_{31}$ (47)		374	390
$O_{34}C_5C_6$ (16)		395	407
$C_{12}N_1N_{30}$, $O_{37}C_{13}C_{14}$, $N_{29}C_2$(40)		420	442
$O_{34}C_5C_6$ (15)	416	459	484
$O_{34}C_5C_6,C_9C_4C_3,C_3N_{32}N_{31}$(42)	469	489	507
$O_{35}C_{10}O_{36}C_{11}$, $H_{26}O_{36}C_{11}C_{10}$(52)	469	499	521
$C_5C_6C_7C_8,C_4C_3N_{32}N_{31}$ (61)		521	544
$C_5C_6C_7,C_{35}O_{11}C_{36}$ (47)		552	575
$H_{15}C_{14}C_{13}N_{29},O_{33}N_{29}N_{31}C_2$ (77)		576	608
$C_{10}O_{34}C_5$, $H_{22}C_6C_5C_4$, $C_5C_6C_7C_8$ (51)	581	583	609
$O_{35}C_{11}O_{36}$, $C_5C_6C_7$, $C_2N_{29}N_{30}$ (36)	581	596	618
$O_{35}C_{11}O_{36},C_{11}C_{10}O_{34}$ (25)	581	603	629
$O_{37}C_{13}C_{14}$ (29)		606	634
$N_{31}C_1N_{30}N_{31}$, $C_{12}N_{31}N_{30}C1$ (68)	609	645	670
$C_{11}C_{10},C_2N_{29}N_{30},C_5C_6C_7$ (41)	646	649	683
$O_{35}C_{10}O_{36}C_{11},H_{26}O_{36}C_{11}C_{10}$ 1C10 (40)	646	672	690
$O_{35}C_{10}O_{36}C_{11},H_{26}O_{36}C_{11}C_{10}$ (42)	646	675	703
$C_2C_{29}C_{30}C$, $O_{33}N_{29}N_{31}C_2$ (56)		729	784
$C_5C_6C7C_8,H_{22}C_6C_5C_4$ (40)		753	799
$C_5C_6C_7,C_5C_6$, $H_{22}C_6C_5C_4$ (39)	753	760	812
$O_{34}C_{16}C_4C_5,H_{22}C_6C_5C_4$ (56)	753	777	823
$C_2N_{29}N_{30}$, $N_{29}N_{30}$ (30)		794	834
$C_{11}C_{10}$ (21),$C_{11}C_{10}$(20),$O_{34}C_5$(36)	804	832	878
$C_{11}C_{10},C_5C_6C_7$(41)	858	873	903
$H_{22}C_6C_5C_4$(68)	858	884	944
$C_4C_3N_{32}$, $N_{29}N_{30},C_5C_6C_7$ (41)	914	919	959
$H_{22}C_6C_5C_4$ (83)	914	962	1015

$H_{15}C_{14}C_{13}N_{29}$, $H_{15}C_{14}H_{17}$, $C_{11}C_{10}$ (43)		963	1028
$H_{22}C_6C_5C_4$,$C_5C_6C_7C_8$ (79)	971	992	1061
$H_{21}C_3N_{32}$ (80)	971	1004	1069
$H_{18}C_{12}H_{20}$, $H_{20}C_{12}C_{13}N_{31}$ (30)		1015	1074
$O_{35}C_{10}O_{36}C_{11}$, $H_{18}C_{12}CN_{31}$ (65)		1022	1077
$H_{15}C_{14}H_{17}$, $H_{15}C_{14}C_{13}N_{29}$ (83)		1045	1086
$H_{22}C_6C_7$,$O_{34}C_{10}$, C_5C_6 (77)	1009	1049	1104
$H_{18}C_{12}CN_{31}$,$H_{18}C_{12}H_{20}$ (83)		1056	1106
$O_{34}C_{10}$,$C_5C_6C_7$ (54)		1065	1132
$N_{29}N_{30}C_1$ (18)		1077	1141
$H_{22}C_6C_7$, C_5C_6 (59)	1073	1127	1143
$H_{15}C_{14}C_{13}N_{29}$,$N_{29}N_{30}$ (42)	1116	1132	1165
$H_{26}O_{36}C_{11}$, $O_{34}C_5$ (67)		1169	1200
$H_{22}C_6C_7$, C_5C_6(87)		1174	1237
$N_{29}C_2$, $N_{29}N_{30}$ (27)		1192	1259
C_4C_3, C_9C_4 (31)	1197	1214	1282
$O_{34}C_5$, $H_{22}C_6C_7$, $H_{27}C_{10}O_{34}$ (55)		1227	1294
$C_2N_{29}N_{30}$, $N_{29}N_{30}$ (23)		1259	1296
$H_{22}C_6C_7$, C_9C_4, $H_{22}C_6C_7$ (64)		1281	1326
$H_{27}C_{10}O_{34}$ (55)		1293	1357
$C_2N_{29}N_{30}$, $H_{27}C_{10}O_{34}$, $N_{29}C_2$ (53)		1298	1368
C_9C_4, C_5C_6 (63)	1302	1324	1407
$C_{35}O_{11}C_{36}$, $H_{26}O_{36}C_{11}$ (67)	1342	1358	1425
$H_{18}C_{12}C_{13}N_{31}$ (61)		1360	1444
$H_{21}C_3N_{32}$ (20)		1374	1453
$H_{18}C_{12}C_{13}N_{31}$ (53)	1381	1391	1466
$H_{18}C_{12}H_{20}$, $H_{21}C_3N_{32}$(63)		1410	1479
$H_{21}C_3N_{32}$, $H_{22}C_6C_7$(43)		1438	1501
$H_{15}C_{14}C_{13}N_{29}$, $H_{15}C_{14}H_{17}$ (96)	1410	1442	1504
$H_{18}C_{12}CN_{31}$, $H_{18}C_{12}H_{20}$ (73)	1410	1445	1513
$H_{15}C_{14}H_{17}$,$H_{15}C_{14}C_{13}N_{29}$ (94)		1456	1516
$H_{18}C_{12}H_{20}$, $H_{22}C_6C_7$ (68)	1457	1459	1518
$H_{18}C_{12}H_{20}$, $H_{22}C_6C_7$, C_5C_6 (49)	1457	1462	1522
$H_{18}C_{12}H_{20}$ (44)	1488	1475	1542
$C_5C_6C_7$,C_5C_6, $H_{22}C_6C_7$, C_5C_6 (85)	1488	1501	1574
$C_5C_6C_7$,C_5C_6, $H_{22}C_6C_7$, C_5C_6 (68)		1584	1668
C_5C_6, C_9C_4 (78)		1621	1702
$N_{30}C_1$, C_5C_6 (63)	1601	1633	1786
$N_{30}C_1$ (69)	1601	1654	1789
$O_{33}C_2$ (76)	1715	1754	1842
$O_{35}C_{11}$(75)	1715	1792	1898
$O_{33}C_2$, $O_{35}C_{11}$ (87)	1715	1794	1905
$C_{12}H_{20}$, $C_{10}H_{27}$ (96)		3018	3044
$C_{14}H_{15}$ (94)		3027	3051
$C_{10}H_{27}$(98)	2933	3040	3082
$C_{12}H_{20}$, $C_{10}H_{27}$ (86)		3075	3105
$C_{10}H_{27}$ (97)		3085	3119
$C_{14}H_{15}$ (99)		3088	3130
$C_{10}H_{27}$(99)		3116	3136
C_3H_{21}, C_6H_{22}, C_7H_{23}, C_8H_{24} (80)		3124	3143
C_3H_{21}, C_6H_{22}, C_7H_{23}, C_8H_{24}, $C_{14}H_{15}$ (90)		3125	3165
C_3H_{21}, C_6H_{22}, C_7H_{23}, C_8H_{24}, C_9H_{25} (92)		3138	3175
C_3H_{21}, C_6H_{22}, C_7H_{23}, C_8H_{24} (97)		3147	3191
C_3H_{21}, C_6H_{22}, C_7H_{23}, C_8H_{24} (80)		3164	3194
C_3H_{21}, C_6H_{22}, C_7H_{23}, C_8H_{24} (99)		3184	3215
$O_{36}H_{26}$ (100)	3226	3712	3907
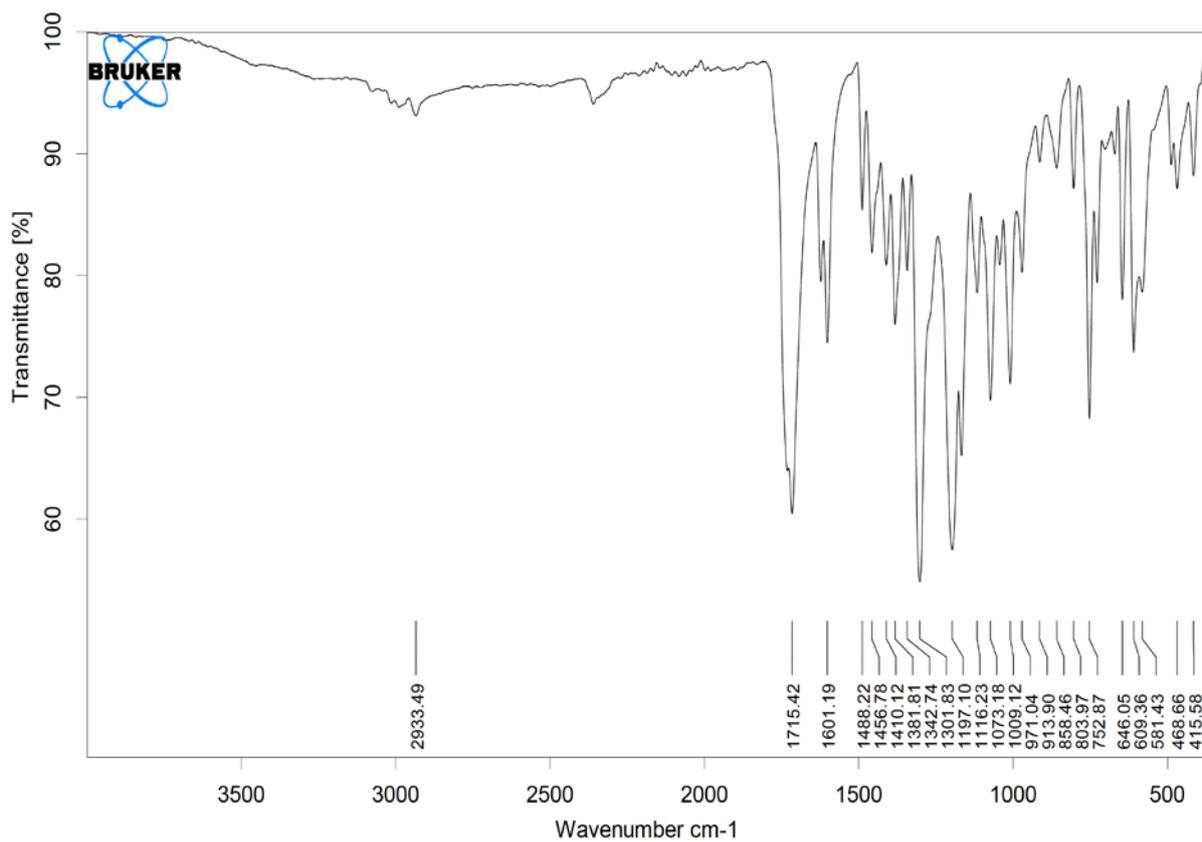
Figure 4. The correlation graphic for vibrational frequencies of the titled compound by using B3PW91, HF and experimental methods, respectively

NMR spectral analysis

It is well known that the combined use of FT-NMR and simulation methods provides a useful approach for the structural prediction of large biomolecules as it is pioneering information to experimental methods (Schlick, 2010). The gauge-independent atomic orbital (GIAO) method which used in the predicting of nuclear magnetic shielding tensors has demonstrated to be quite accurate and accepted from scientific community, in particular when applied in the context of highly correlated ab initio methods.

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 (Wade, 2006; Rani et al., 2010; Subramanian et al., 2010). In this framework, the optimized molecular geometry of the molecule was obtained by using B3PW91 and HF methods with the 6-311+G (d,p) basis set 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 (Table 4). Theoretical and experimental 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 (Figure 5).

Table 4. Experimentally and theoretically ^{13}C and ^{1}H-NMR (B3PW91/(DMSO) and HF/(DMSO)) chemical shift values of the studied molecule according to the TMS standard (⧫/ppm)

No	Experim.	DFT/6311d/DMSO	Fark/DMSO	HF/6311d/DMSO	Fark/DMSO
C1	146.81	155.62	-8.81	162.94	-16.13
C2	151.28	155.29	-4.01	161.26	-9.98
C3	149.29	159.19	-9.90	168.24	-18.95
C4	122.01	131.89	-9.88	133.49	-11.48
C5	157.49	165.54	-8.05	167.84	-10.35
C6	121.62	131.41	-9.79	134.48	-12.86
C7	125.87	138.38	-12.51	146.83	-20.96
C8	113.15	130.35	-17.20	134.57	-21.42
C9	133.37	142.51	-9.14	149.65	-16.28
C10	65.25	73.61	-8.36	70.52	-5.27
C11	168.35	179.56	-11.21	180.49	-12.14
C12	13.96	13.18	0.78	18.77	-4.81
C13	165.94	172.09	-6.15	176.11	-10.17
C14	23.40	26.09	-2.69	30.36	-6.96
H15	2.49	2.71	-0.22	2.84	-0.35
H16	2.49	2.68	-0.19	2.82	-0.33
H17	2.49	2.13	0.36	2.35	0.14
H18	2.35	2.25	0.10	2.57	-0.22
H19	2.35	2.53	-0.18	2.78	-0.43
H20	2.35	2.55	-0.20	2.76	-0.41
H21	9.94	10.48	-0.54	10.13	-0.19
H22	7.95	7.84	0.11	8.24	-0.29
H23	7.12	7.75	-0.63	8.24	-1.12
H24	7.09	7.53	-0.44	7.90	-0.81
H25	7.51	7.76	-0.25	8.29	-0.78
H26	11.77	6.75	5.02	6.59	5.18
H27	4.97	4.99	-0.02	4.92	0.05
H28	4.97	4.39	0.58	4.08	0.89

The obtained R^2 value was found close to 1 especially for ^{13}C-NMR data (Figure 5).

Nonlinear Optical Properties

The nonlinear optical activity provide useful information for frequency shifting, optical modulation, optical switching and optical logic for the developing technologies in areas such as communication, signal processing and optical interconnections (Andraud et al., 1994; Geskin et al., 2003). In the presence of an applied electric field, the energy of a system is a function of the electric field.
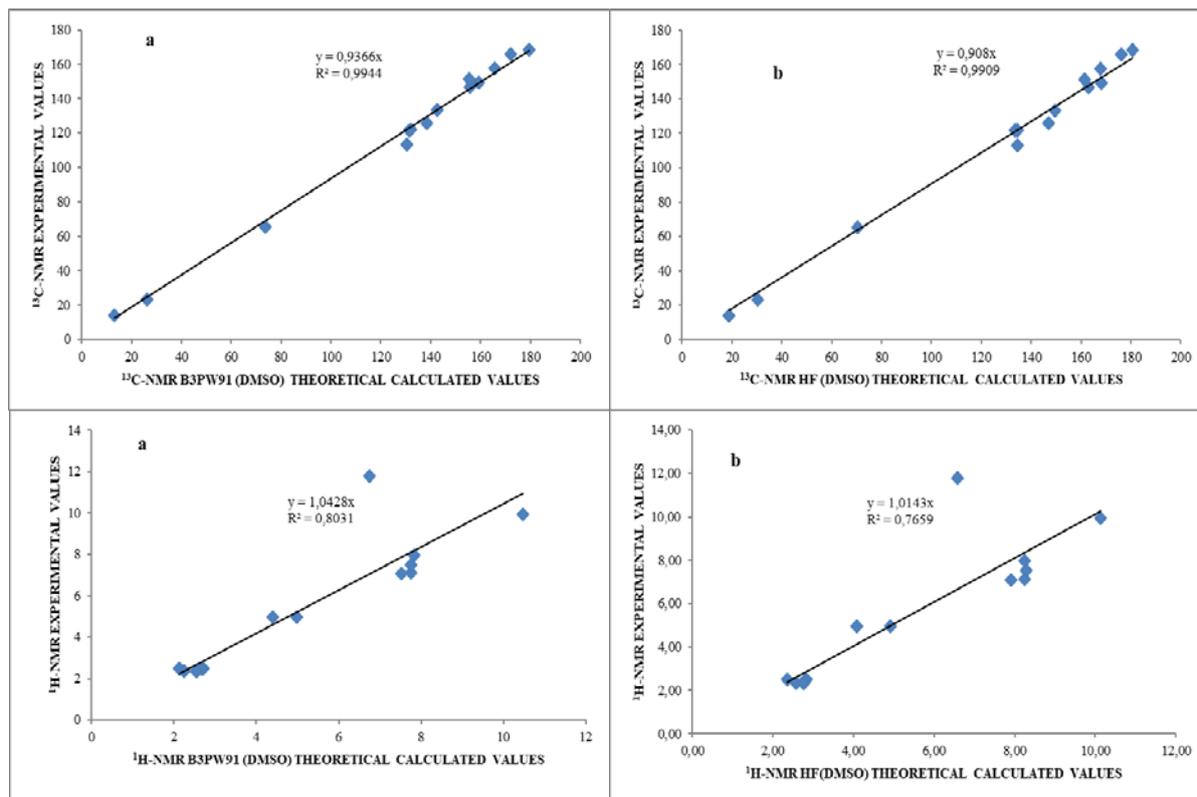
Figure 5. Regression analysis of the theoretical values calculated with experimental data using the least squares method of ^{13}C-NMR and ^{1}H-NMR chemical shift values by B3PW91 and HF methods 6-311+G (d.p) basis set

First hyperpolarizability is a third rank tensor that can be described by a 3 x 3 x 3 matrix. The 27 components of the 3D matrix can be reduced to 10 components due to the Kleinman symmetry (Kleinman, 1962). The total static dipole moment μ, the mean polarizability α_0 and the mean first hyper polarizability β_0, using the x-, y- and z- components are defined as

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

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

The dipole moment, the mean polarizability α_0 are calculated using Gaussian09 software and is found to be 3.088 Debye and 23.334×0^{-23} e.s.u respectively. The first order hyper polarizability β was also calculated using the finite field approach theory. The components of first hyperpolarizability can be calculated using the following equation:

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

Where, the total static dipole moment (μ), linear polarizability (α) and the first hyperpolarizability (β) using the *x*, y, *z* components are defined as (Karamanis et al., 2008). 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/6-311G(d) level of theory (Govindarajan et al., 2012) (Table 4).

The nonlinear optical properties of the molecule; nonlinear optical properties after calculating the polar ΔE energies in the single point energy calculation; polarizability and hyperpolarizability values were calculated by making polar calculations in single point energy calculation (Table 5).

Table 5. Calculated dipole moment, polarizability and hyperpolarizability values of the molecule by B3PW91 and HF methods 6-311+G (d.p) basis set

B3LYP		HF	
μ_x	-5.2457 debye	μ_x	-5.6150 debye
μ_y	2.6625 debye	μ_y	2.9745 debye
μ_z	-0.3772 debye	μ_z	-0.9031 debye
μ_{Toplam}	5.8948 debye	μ_{Toplam}	6.4180 debye
α_{xx}	47.202 a.u.	α_{xx}	38.194 a.u.
α_{yy}	34.049 a.u.	α_{yy}	29.880 a.u.
α_{zz}	19.364 a.u.	α_{zz}	18.451 a.u.
α	33.538×10^{-24} esu	α	28.842×10^{-24} esu
$\Delta\alpha$	24.121×10^{-24} esu	$\Delta\alpha$	17.169×10^{-24} esu
β_x	-2617.136 a.u.	β_x	-841.551 a.u.
β_y	3114.727 a.u.	β_y	1895.851 a.u.
β_z	759.225 a.u.	β_z	224.924 a.u.
β_{xxx}	-1630.659 a.u.	β_{xxx}	193.446 a.u.
β_{xxy}	-428.744 a.u.	β_{xxy}	-579.652 a.u.
β_{xyy}	-557.733 a.u.	β_{xyy}	-455.344 a.u.
β_{yyy}	1487.295 a.u.	β_{yyy}	398.686 a.u.
β_{xxz}	1212.979 a.u.	β_{xxz}	1053.480 a.u.
B_{xyz}	414.452 a.u.	B_{xyz}	443.685 a.u.
B_{yyz}	896.797 a.u.	B_{yyz}	501.386 a.u.
β_{xzz}	-218.536 a.u.	β_{xzz}	-228.854 a.u.
β_{yzz}	80.964 a.u.	β_{yzz}	-47.609 a.u.
B_{zzz}	334.384 a.u.	B_{zzz}	169.803 a.u.
β	4.139×10^{-30} esu	β	2.086×10^{-30} esu

Conclusion

The theoretical study, All quantum chemical calculations were carried out by using Gaussian 09W program package and the GaussView molecular visualization program. The electronic properties were calculated by applying the 6-311G+(d,p) diffused and polarized basis set and the B3LYP and HF methods to 2-[1-acetyl-3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide. Theoretically, HOMO-LUMO energies were created. Electronic parameters such as I; Ionization potential, A; electron affinity, η; molecular hardness, S; molecular softness and χ; electronegativity, total energies, dipole moment values were determined from HOMO-LUMO energies. From the obtained molecular energy potential shape, it was observed that the negative charge covers the heteroatoms and the positive region is above the remaining groups. Vibration frequencies and vibration spectra to determine the functional groups in the structure titled compound calculated the same methods. the optimized molecular geometry of the molecule was obtained according to The gauge-independent atomic orbital (GIAO) method in DMSO solvent. Theoretical and experimental 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. Finally, the nonlinear optical properties of the related compound were calculated theoretically. Urea (0.37×10^{-30} esu) is used as a standard substance in compounds with non-linear optical properties. It has been observed that the related molecule has a higher hyperpolarizability value than urea.

Scientific Ethics Declaration

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

Acknowledgements or Notes

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Author Information

Murat BEYTUR	Haydar YÜKSEK
Kafkas University	Kafkas University
,Kars, Turkey	Faculty of Science and Letters, Department of Chemistry,
Contact E-mail: *muratbeytur83@gmail.com*	Kars, Turkey

To cite this article:

Beytur, M. & Yüksek, H. (2022). Density functional theory and ab initio hartree-fock computational study 2-[1-acetyl-3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acide. *The Eurasia Proceedings of Science, Technology, Engineering & Mathematics (EPSTEM), 20,* 30-42.