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ABSTRACT

In the present work novel conjugate of gallic acid (1) have been synthesized, which was isolated from fruits of Phyllanthus emblica Linn, commonly known as Indian gooseberry or Amla. Gallic acid was methylated to 3,4,5 trimethoxy gallic acid (2), which then underwent steglich esterification with vaniline to (3) yield 4formyl-2-methoxyphenyl 3,4,5- trimethoxybenzoate. The synthesized compounds have been characterized with the help of ¹H NMR, ¹³C NMR, UV, FT-IR and mass spectroscopy. Density functional theory (DFT/B3YLP) using 6-31G (d,p) basis set have been used for quantum chemical calculations. Intramolecular interactions have been analyzed by AIM (Atom in molecule) approach. The electronic properties such as HOMO and LUMO energies and frontier orbital energy gap were calculated by TD-DFT approach. The reactive site and reactivity within the molecule were examined by reactivity descriptors such as global and local reactivity descriptors. The electrophilic and nucleophilic reactivity have been determined by molecular electrostatic potential (MEP) experiment. Dipole moment, m polarizability and first hyperpolarizability values have calculated to depict the nonlinear optical property of the synthesized compound.

Keywords: Gallic acid, trimethoxy gallic acid, steglich esterification, MEP, NLO and AIM.

INTRODUCTION

Plant products have been since time immoral as a source of folk medicine. Drugs isolated directly from natural sources have been used as 'lead' compound for the synthesis of newer drugs sometimes with high biological efficacy and higher yield. *Emblica officinalis* Gaertn or *Phyllanthus emblica* Linn, commonly known as Indian gooseberry or Amla, is arguably the most important medicinal plant in the Indian traditional system of medicine, the Ayurveda (Vasudevan et al 2007) "Amla" is a deciduous tree *Emblica officinalis* is gift of nature to mankind. It is highly nutritious and is one of the richest sources of vitamin C, amino acids and minerals. Many pharmacological studies of the fruit have shown its antioxidant, anticarcinogenic, antitumor, antigenotoxic, antiinflamatory activities supporting its traditional uses as adaptogenic, cardioprotective, gastroprotective, antianemia, antihypercholesterolemia, cytoprotective, memory enhancing activity and neuroprotective. In recent years drugs isolated directly from natural source have been used as 'lead' compound for the synthesis of newer drugs sometimes with high biological efficacy and higher yield. The present work aims in the synthesis of prodrug 4-formyl-2-methoxyphenyl 3,4,5-trimethoxybenzoate (**3**) using DCC as coupling reagent and DMAP as catalyst

Srivastava et al. 2016) Trimethoxy gallic acid (2) needed for synthesis of the present compound (3) was derived from biologically active constituent gallic acid (1) isolated from *Phyllanthus emblica*.

Synthesis of compound (3) is given in **scheme 1.** The structure of the synthesized compound was characterized with the help of ¹H, ¹³C NMR, UV, IR and mass spectrometry. The molecular geometry of the synthesized compound was studied with the help of density functional theory (DFT) with B3LYP/6-31G (d, p) basis set. Intramolecular interactions have been analyzed by AIM (Atom in molecule) approach. The electronic properties such as HOMO and LUMO energies and frontier orbital energy gap were calculated by TD-DFT approach. The reactive site and reactivity within the molecule were examined by reactivity descriptors such as global and local reactivity descriptors. The electrophilic and nucleophilic reactivity have been determined by molecular electrostatic potential (MEP) experiment. Dipole moment, m polarizability and first hyperpolarizability values have calculated to depict the nonlinear optical property of the synthesized compound.



Scheme 1: A) (CH₃)₂SO₄; B) 3-OH-4-OCH₃C₆H₅CHO/DCC/DMAP, stirred at room temperature.

MATERIAL AND METHODS

Materials and physical measurements

All reagents for synthesis were purchased from Sigma Aldrich (St. Louis, MO) and used without further purification. Thin layer chromatography (TLC) was performed on silica gel G coated plates to detect completion of reaction. Compounds were purified by column chromatography using silica gel (60-120 mesh). ¹H NMR spectrum was recorded on Bruker DRX-300 MHz spectrometer using CDCl₃ and DMSO as the solvent and TMS as an internal standard, chemical shift was reported as δ (ppm) and ¹³C NMR spectra were recorded on JOEL AL 300 FTNMR (75Mz) using TMS as an internal reference. FT-IR spectra were recorded on Perkin Elmer FT-IR spectra were recorded on Agilent 6520 Q–TOF mass spectrometer. Ultraviolet absorption spectra were obtained (in the range of 200-500 nm) using ELICO BL-200 UV-Vis spectrophotometer equipped with a 10 mm quartz cell in chloroform.

Extraction and isolation of gallic acid

For the preparation of extract of the fruit of *Phyllanthus emblica* was done as reported earlier (Zhang et al. 2014). Dry butanol extract (2 gm) of the fruit of *Phyllanthus emblica* was subjected to column chromatography using silica gel (60-120 mesh) and started by chloroform solvent and further polarity was enhanced using Chloroform/ methanol (98:2- 92:8) afforded 15 fractions, out of which 8 fractions contained 1 in impure form. Compound **1** (80mg) was obtained in pure form with repeated column chromatography using chloroform/methanol in increasing polarity. Molecular formula: $C_7 H_6 O_5$ ¹H NMR (300 MHz, CDCl₃) δ (ppm): 7.37 (2H, s, H-2 H-6), ESI-MS: m/z 171 [M⁺+1]. The isolated gallic acid was further identified by authentic sample.

Synthesis of 3,4,5-trimethoxygallic acid

70 mg (0.41 mmol) of gallic acid was dissolved in 10 ml NaOH (8gm NaOH dissolved in 50ml water). The flask was immediately stoppered, and then reaction mixture was shaken occasionally until all the acid was dissolved, 1 ml of dimethyl sulphate was then added and the flask was stirred for 1 hour, during this temperature was maintained below 30-35 C. The flask was then fitted with a reflux condenser and reflux for 2 hour. The ester thus produced was saponified by addition of 20 mg of sodium hydroxide dissolve in 2 ml of water and refluxing for two hours. The reaction was monitored by TLC. The reaction mixture was then cooled and acidified with dilute HCl, the precipitated 3,4,5-trimethoxybenzoic acid (**2**) was filtered and washed with cold water. Trimethylated gallic acid (**2**) thus obtained was 110mg. Molecular formula: $C_{13} H_{12} O_8^{-1} H NMR$ (300 MHz, CDCl₃) δ (ppm): 3.93(9H, s, OCH₃).

Synthesis of 4-formyl-2-methoxyphenyl 3,4,5-trimethoxybenzoate

100mg (0.47 mmol) of **2** and 50 mg of vanilline was dissolved in 15 mL of dioxane and then DCC (55 mg, 0.266 mmol) and DMAP (33 mg, 0.270 mmol) were added. The reaction mixture was stirred at room temperature. The completion of reaction was monitored with the help of thin layer chromatography (TLC). Reaction mixture was washed with 5% HCl, water and dried over anhydrous sodium sulphate and filtered. The organic layer was concentrated under reduced pressure and purified by column chromatography using ethyl acetate: hexane (15:85) yielding compound **3** 100 mg (83.33%) as viscous. Molecular formula: $C_{18}H_{18}O_7$, ¹H NMR(300MHz, CDCl₃) δ (ppm): 9.61 (1H, s,CHO17), 7.44 (1H,d, H16), 742(1H, d, H15), 7.06 (1H, d, H13), 7.03 (1H, s, H6 & H2), 3.97(9H, s,OCH3-7, OCH3-8 & OCH3-9) 3.91(3H, s, OCH3-10) ¹³C NMR(75 MHz, CDCl₃) δ (ppm): 190.97 (C17), 160.51 (C10) 151.65 (C3,C5,C12) 147.11(C4 & C11), 129.84 (C14 & C16), 127.61 (C1 & C15), 114.33 (C13), 108.67 (C2 & C6), 56.11(C7,C8,C9 & C18) (ESI-MS: m/z 347[M⁺+1], IR vmax (in cm⁻¹): 2924, 2852, 1660, 1510, 1463, 1431, 1377, 1298, 1267, 1201, 1172, 1155, 1126.

Computational methods

All the calculations of synthesized compound was carried out with help of Gaussian 09 program package (Frisch et al 2009) using B3LYP functional and 6-31G (d, p) basis set. UV-Vis spectra, electronic transitions and electronic properties such as HOMO-LUMO were computed with the help of time-dependant DFT (TD-DFT) method. The molecular structures were visualized with the help of Gauss View (Gauss et al 2009). AIM calculations were performed by AIMALL program (Keith et al 1997)

RESULT AND DISCUSSION

¹H and ¹³C NMR Spectroscopy

The experimental and calculated value of ¹H & ¹³C NMR chemical shifts of **3** are given in **Table 1**. In the ¹H NMR of compound **3 one** proton singlet observed at δ 9.61 was of aldehyde group of vanilline. Further aromatic proton at H-15 and H-16 of vanillin moiety were observed at δ 7.44 and δ 7.42 respectively as doublet (J=6Hz). A singlet of H-13 of vanillin appeared at δ 7.06. Two singlets one of three protons and other of nine protons were observed at δ 3.91 and δ 3.97 respectively.

The singlet at δ 3.91 was due to methoxy group (18-OCH₃) of vanillin and the peak at δ 3.97 is probably due to three methoxy groups (7-OCH₃, 8- OCH₃,9- OCH₃) of **2.** Another singlet of two protons at δ 7.03 was observed due two equivalent protons at H-2 and H-6. All the values of¹ H NMR were comparable with the theoretical values. In the ¹³CNMR signal for C-10 carbon of the ester moiety was observed at δ 163.28. The signals for C-2 and C-6 carbons (equivalent carbons) appeared at same chemical shift δ 127.61. Carbon signal for methoxy groups at C-7, C-8, C-9 and C-18 were observed at δ 56.11. Other signal of vanillin moiety and methylated gallic acid were also observed indicating esterification of trimethoxy gallic acid with vanillin. All these values correlated with the theoretical values.

UV–Vis absorption spectra

Theoretical calculations of UV-Vis absorption spectra were done with the help of TD-DFT method on B3LYP/6-31G (d, p) level. The experimental absorption wavelengths (energies) and computed electronic values, such as absorption wavelength (λ), energy gap (E), Oscillator strength (f), and assignments of electronic transitions are mentioned in **Table 2**. The molecular orbital diagram of compound **3** is shown in **Fig. 1**). Experimental UV for compound **3** showed four electronic transitions at 326 nm, 295nm, 265nm and 226 nm corresponding to theoretical values at 326 nm, 283nm, 265nm and 222 nm.

	¹³ C NMR			¹ H NMR		
	Calculated	Experimental	Atom No	Calculated	Experimental	
C-1	124.31	127.61	CHO17(s)	9.96	9.83	
C-2	107.35	108.67	H-16(d)	8.55	7.445	
C-3	152.88	151.65	H-15(d)	7.64	7.425	
C-4	142.93	147.11	H-6	7.60	7.03	
C-5	152.38	151.65	H-2	7.46	7.03	
C-6	106.53	108.67	H-13	7.25	7.06	
C-7	56.39	56.11	90CH3(s)	3.82	3.97	
C-8	59.93	56.11	7OCH₃(s)	3.81	3.97	
C-9	56.32	56.11	80CH ₃ (s)	3.76	3.97	
C-10	160.51	163.28	180CH ₃ (s)	3.89	3.91	
C-11	145.74	147.11				
C-12	148.61	151.65				
C-13	125.32	114.33				
C-14	131.19	129.84				
C-15	108.20	127.61				
C-16	120.65	129.84				
C-17	184.39	190.97				
C-18	56.54	56.11				

Table 1. Experimental and calculated ¹H and ¹³C NMR of 3.

Table 2. Electronic transitions (calculated and experimental).

Major contributing	ΔE (eV)	Calculated	Assignment	Observed
Molecular orbitals		(λ _{max})		(λ _{max})
H→L (38.94%)	4.22	326.55	n →π*	326.01
H-1→L+1 (39.48%)	4.91	283.46	n →π*	295.76
H-3→L (33.27%)	5.14	265.61	$\pi \rightarrow \pi^*$	265.51
H→L+2 (44.90%)	5.99	222.63	$\pi \rightarrow \pi^*$	226.20



Figure 1. Molecular orbital diagram of compound 3.

The electronic transition at 326 nm may be attributed mainly due to $H\rightarrow L$ transition with 38.94% major contribution, which was assigned due to $n \rightarrow \pi^*$ transition, 295nm may be attributed due to $H-1\rightarrow L+1$ with 39.48% major contribution which was assigned due to $n \rightarrow \pi^*$ transition, 265nm may be attributed due to $H-3\rightarrow L$ with 33.27% contribution which was assigned due to $\pi \rightarrow \pi^*$ while electronic transition at 226 nm were attributed mainly to $H\rightarrow L+2$ transition with 44.90% major contribution which was assigned due to $\pi \rightarrow \pi^*$ transition.

Global reactivity descriptors

The chemical reactivity of the molecular systems has been determined by the conceptual density functional theory (Parr et al 1989). Electronegativity (χ), chemical potential (μ), global hardness (η), global softness (S) and electrophilicity index (ω) are global reactivity descriptors, highly successful in predicting global reactivity trends. On the basis of Koopmans's theorem, (Koopmans et al 1934) global reactivity descriptors are calculated using the energies of frontier molecular orbitals ϵ_{HOMO} , ϵ_{LUMO} as $\chi = -1/2(\epsilon_{LUMO} + \epsilon_{HOMO})$, $\mu = -\chi = -1/2(\epsilon_{LUMO} + \epsilon_{HOMO})$ $1/2(\epsilon_{LUM0} + \epsilon_{HOM0})$, $\eta = 1/2(\epsilon_{LUM0} - \epsilon_{HOM0})$, $S = 1/2\eta$ and $\omega = \mu^2/2\eta$. The energies of frontier molecular orbitals (ϵ_{HOMO} , ϵ_{LUMO}) and global reactivity descriptors for **2** are listed in **Table 3**. The frontier orbital gap helps to characterize molecular electrical transport properties (Fleming et al 1976' Fukui 1982'Singh et al 2016) the chemical reactivity and kinetic stability of the molecule. A molecule with a small frontier orbital gap is generally associated with a high chemical reactivity and low kinetic stability. The frontier orbital energy gap for compound 3 was found to be 4.304. Larger the HOMO-LUMO energy gap, harder the molecule. The HOMO-LUMO energy gap of compound 3 was slightly lower, signifying lower excitation energy .When two molecules react, which one will act as an electrophile or nucleophile will depend upon the value of electrophilicity index. Higher the value of the electrophilicity index better is the electrophilic character. Thus compound acts as a good electrophile as the molecule shows higher value for global electrophilicity index (ω) at 4.304 eV.

Table 3. Calculated ε_{HOMO} , ε_{LUMO} , energy band gap ($\varepsilon_L - \varepsilon_H$), chemical potential (μ), electronegativity (χ), global hardness (η), global softness (S), global electrophilicity index (ω) for compound 3



Figure 2. Molecular electrostatic potential of compound 3.

Molecular Electrostatic Potential

Molecular electrostatic potential surface (MEP) for the compounds **3** was calculated by DFT/B3LYP at 6-31G (d, p) basis set and MEP surface are plotted in **Fig. 2**. The MEP is a plot of the electrostatic potential mapped onto the constant electron density surface. It simultaneously displays the molecular shape, size, and charge distribution, as well as reactive sites of a molecule (Srivastava et al. 2016, Alkorta et al. 1996, Scrocco et al 1978, Luque et al. 1993). The red and yellow regions of the MEP are related to electrophilic reactivity and the blue regions to nucleophilic reactivity (Powell et al 2004). In compound **3** the carboxyl group is characterized by red region indicating relative surplus of electrons and may be a site for electrophilic interactions. There by confirming that carboxyl group at C-10 in **2** was esterified leading to the synthesis of ester **3**.

Non -linear optical analysis

The non- linear optical properties of an organic moiety have been availed for optical switching, fibre-optic communication and optical data storage (Zhou et al 2005) in photonics technologies(Kaya et al) in areas such as signal processing telecommunications and optical inter connections. Therefore in order to probe the molecular structure and NLO response, the first order hyperpolarizability, of the novel molecular system and its associated (μ) and (α) are calculated using B3LYP/6-31G (d,p) basis set from Gaussian 09W program.

The mathematical figuring of magnitude of total static dipole moment (μ_{tot}), isotropic polarizability (α_0), and first hyperpolarizability (β_0) from entire equations using the x,y,z components is as summarised below.

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)$$

$$\alpha_0 = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}$$

And

$$\beta_0 = \left(\beta_x^2 + \beta_y^2 + \beta_z^2\right)^2$$
$$\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$$
$$\beta_y = \beta_{yyy} + \beta_{xxy} + \beta_{yzz}$$
$$\beta_z = \beta_{zzz} + \beta_{xxz} + \beta_{yyz}$$

Since the value of the polarizability (α_0), first hyperpolarizability (β_0) of Gaussian output are displayed in atomic unit (a.u.) and these values are altered into electrostatic unit (esu) using converting factors as (for α_0 : 1 a.u. = 0.1482 x 10⁻²⁴ esu; for β_0 : 1 a.u = 0.008639 x 10⁻³⁰ esu). The total static dipole moment and mean first hyperpolarizability of **3** was found to be 3.325 Debye and 22.614× 10⁻³⁰ esu respectively, as shown in **Table 4**. which is greater than that of the standard NLO material urea (the β_0 of urea 0.13 ×10⁻³⁰ esu) (Adant et al 2004). Thus it is deduced that compound **2** may act as good NLO object in future and show optical properties.

Tabla 1	Coloulated D	n alma a m a n t/	··· \ Delewinehilit	/ Lev \ E:mail	. I ly man malanina h		f common and 2
i able 4.	Calculated Di	pointoment	μ_0 , Polarizabilit	$(\alpha_0), risc$. пурегројанzа.	μπ ι γ (0 ₀) Ο	i compound 5.

Dipole moment			Hyper Polarizability
μх	2.5940	βxxx	-2321.58
μγ	1.2193	βxxy	-595.775
μz	1.6866	βxyy	-145.263
μ	3.3257	βγγγ	-215.981
Pol	arizability		
αχχ	348.917	βxxz	9.06760
αγγ	1.28526	βxyz	10.0519
αzz	242.009	βyyz	61.3392
		βxzz	-20.6815
		βyzz	2.09733
		βzzz	21.7538
<α>	29.2552	βtotal(esu)	22.6142

AIM approach

Topological parameters are useful tool to characterize the strength of hydrogen bond. The geometrical criteria for the existence of hydrogen bond are as follows: (i) the distance between proton (H) and acceptor (A) should be less than the sum of the Van der Waal's radii of these atoms.

(ii) The angle between 'donor (D), proton (H) and acceptor (A)' should be greater than 90°. (iii) There should be elongation of 'donor (D) proton (H)' bond length. As the above criteria were often considered insufficient, hence the existence of hydrogen bond was supported further by Koch and Popelier criteria (Kleinman 1962) based on 'Atoms in Molecules' theory (i) the existence of bond critical point for the 'proton (H).....acceptor (A)' contact as a confirmation of the existence of hydrogen bonding interaction. (ii) The value of electron density (ρ H. . . A) should be within the range 0.002–0.040 a.u. (iii) The corresponding Laplacian $^{2}\rho$ (r_{BCP}) should be within the range 0.024-0.139 a.u. (Murray et al 1996). According to (Rozas et al. 2004) the interactions may be classified as follows: (i) strong H-bonds are characterized by $\nabla^2 \rho_{(BCP)} < 0$ and $H_{BCP} < 0$ and their covalent character is established. (ii) Medium H-bonds are characterized by $\nabla^2 \rho_{(BCP)} > 0$ and $H_{BCP} < 0$ and their partially covalent character is established. (iii) Weak H-bonds are characterized by $\nabla^2 \rho_{(BCP)} > 0$ and $H_{BCP} > 0$ and they are mainly electrostatic. The weak interactions are characterized by $\nabla^2 \rho_{(BCP)} > 0$ and $H_{BCP} > 0$ and the distance between interacting atoms is greater than the sum of Van der Waal's radii of these atoms. Molecular graph of the compound 3 using AIM program at B3LYP/6- 31G (d,p) level is presented in Fig.3. The topological parameters for bonds of interacting atoms are given in **Table 5**, on the basis of above criteria, as $\nabla^2 \rho$ (BCP) and H_{BCP} parameters were greater than zero hence H36......H38, 09......H30,O24......H34 are weak interactions. In this article, the Bader's theory application was used to estimate hydrogen bond energy (E). Espinosa proposed proportionality between hydrogen bond energy (E) and potential energy density (V_{BCP}) : $E = 1/2(V_{BCP})$ (Espinosa et al.1998). According to AIM calculation, the total energy of intramolecular interactions was calculated as -0.009387 kcal/mol.

Table 5. Topological parameters for intramolecular interaction in compund; electron density (ρ_{BCP}), Laplacian of electron density ($\nabla^2 \rho_{BCP}$), electron kinetic energy density (G_{BCP}), electron potential energy density (V_{BCP}), total electron energy density (H_{BCP}), Hydrogen bond energy (E_{HB}) at bond critical point (BCP).

Interactions	$\boldsymbol{\rho}_{BCP}$	$ abla^2 ho_{BCP}$	G _{BCP}	V _{BCP}	H _{BCP}	E _{HB}
H36…H38	0.000147	0.000700	0.000121	-0.000066	0.000055	-0.000033
O9H30	0.015766	0.059745	0.013234	-0.011533	0.001701	-0.0057665
O24H34 0.009712 0.059745 0.008393 -0.007175 0.001218 -0.0035875						
$\rho_{BCP}, \nabla^2 \rho_{BCP}, G_{BCP}, V_{BCP}, H_{BCP}$ in a.u. and E_{HB} in (kcal/mol)						



Figure 3. Molecular graph of compound 3 using AIM program ring critical point (red spheres) and bond path (pink lines).

Vibrational spectral analysis

An experimental FT-IR spectrum of synthesized compound has been recorded in the range of 4000–450 cm⁻¹ The calculated and experimental FT-IR wave numbers for **3** with their assignments are given in **Table 6**. The calculated wave numbers are scaled down by a single scaling factor 0.9608 (Sundraganesan et al. 2009). The position of carbonyl group C=O stretching vibration is determined by factors like conjugation, ring strain, hydrogen bonding and physical state. These factors give particulars about the environment of C=O group.

Generally C=O stretching vibrations appear in the region of 1870–1540 cm⁻¹ (Srivastava et al. 2017, Silverstein et al.1963). In the spectrum of compound **3**, the stretching vibrations of carbonyl group C=O (C8-O9) observed at 1680 cm¹ where as calculated value was found at 1631 cm⁻¹. Stretching vibrations of C-O (C10-O7) observed at 1172cm⁻¹ whereas its theoretical value was observed at 1171 cm⁻¹ thus confirms the ester linkage at C-10. The C-H symmetric stretching vibration of methyl proton of methoxy group of trimethoxygallic acid and vanillin were observed at 2924 cm⁻¹ and 2852 cm⁻¹ respectively. In aromatic hydrocarbon, C=C stretching vibrations within the ring are observed in the region between 1566-1510 cm⁻¹ (Krishnakumar et al. 2008). In the spectrum of compound **3**, C=O (C16-O17) of aldehydic group of vanillin was observed at 1666 cm⁻¹ whereas its theoretical value was observed at 1719 cm⁻¹. The stretching vibration of C=O (C11-O22) of methoxy group of vanillin was observed at 1298 cm⁻¹ and the calculated value was found to be 1323 cm⁻¹, thus confirming esterification of vanillin with trimethoxygallic acid. Besides these values various bending vibrations were also observed.

Experimental	Calculated	Assignments
2924	2960	C21H37 (C-H) stretching
2852	2791	C16H31(C-H) stretching
1680	1731	O9C8 (C=O) ester stretching
1666	1719	O17C16 (C=O) CHO stretching
1566	1581	C=C (aromatic) stretching (vanillin)
1510	1484	C=C (aromatic) stretching (trimethoxy gallic acid)
1463	1483	C6H27 (C-H) bending
1431	1438	C19H33 (C-H) bending
1377	1374	C16H31 (C-H) bending
1298	1323	O22C11 (C=0) stretching (OCH3)
1267	1246	C12H28 (C-H) bending
1201	1193	C15H30 (C-H) bending
1172	1171	C1007 (C-O) ester stretching
1155	1157	C25H41 (C-H) bending (OCH3)
1126	1125	C9H33 (C-H) bending
1040	1037	O24C25 (C=O) stretching

Table 6. Experimental and selected theoretical vibration wave numbers (cm⁻¹) of compound 2.

CONCLUSION

Synthesis of compound **3**, a derivative of methylated gallic acid was carried out by using Steglich method and was obtained in high yield. The gallic acid used was isolated from fruits of *Phyllanthus emblica* in good yield. The synthesized compound **3** was characterised with the help of ¹H, 1³C NMR, FT-IR, UV-visible spectroscopy and mass spectrometry. Theoretical analysis performed with the help of density functional theory using B3LYP functional and 6-31-G (d, p) basis set has supported experimental results. High value for global electrophilicity index (34.304 eV) for compound **3** suggest it to be a good electrophile. Intramolecular Hydrogen bonding interactions and ellipticity as probed by AIM approach illustrated weak hydrogen bonds and π -character of bonds in the aromatic ring (Andriana et al. 2017). On the basis of first hyperpolarizability analysis we conclude that investigated molecule may be used as good non-linear optical material and show optical responses.

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