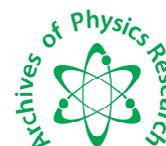




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CODEN (USA): APRRC7

### Molecular Structure, Vibrational Spectra of Glycozolidal (2, 7-dimethoxy-9H-carbazole-3-carbaldehyde, C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>), Using Density Functional Theory

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#### ABSTRACT

*This work is devoted to theoretical study on molecular structure of glycozolidal. The equilibrium geometry, harmonic vibrational frequencies and infrared intensities were calculated by density functional B3LYP methods with the LanL2DZ basis set and were interpreted in terms of potential energy distribution (PED) analysis. The internal coordinates were optimized repeatedly for many times to maximize the PED contributions. The thermodynamic functions and electronic properties of the title compound were also performed at B3LYP/ LanL2DZ level of theory.*

**Keywords:** PED, Glycozolidal, Molecular structure, Vibrational Spectra, Electronic Properties.

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#### INTRODUCTION

Natural products have been the subject of investigation for many reasons. They have got wide applications, such as antibiotics, pharmacologically active agents or are otherwise of interest in human or animal medicine. They hold great potential as probes of the cellular processes in which they interfere. Structural and conformational studies lead to the hypothesis concerning target ligand interactions while synthesis is a means to test this hypothesis by a total synthesis of derivatives [1,2]. The title compound known as glycozolidal (2,7-dimethoxy-9H-carbazole-3-carbaldehyde), C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>, is a naturally occurring carbazole, which was isolated from the roots of *Clausena lansium*. Carbazole alkaloids are major compounds found in Rutaceae plants, especially in *Clausena* genus, which showed diverse pharmacological activities such as anti-cancer, anti-malaria, anti-TB and anti-HIV properties [3].

To the best of our knowledge neither the vibrational analysis nor the comparative quantum chemical calculations for glycozolidal have been reported so far in the literature. Therefore, the aim of this paper is to interpret the theoretically calculated vibrational spectra of the glycozolidal by means of the potential energy distribution (PED) analysis of all fundamental vibrational modes. In this regard, with the help of VEDA program both the PED analysis and its optimization were carried out [4].

## MATERIALS AND METHODS

*Structure*

The crystal structure of the title compound glycozolidal is taken from the work of H. K. Fun *et al* [3]. The molecular structure using numbering scheme of the title compound is given in fig 1 and the structure as viewed by Gaussian software is shown in fig 2. The experimental FTIR or Raman spectra of the compound are not yet reported so here the theoretically plotted FTIR spectra are shown in fig 3.

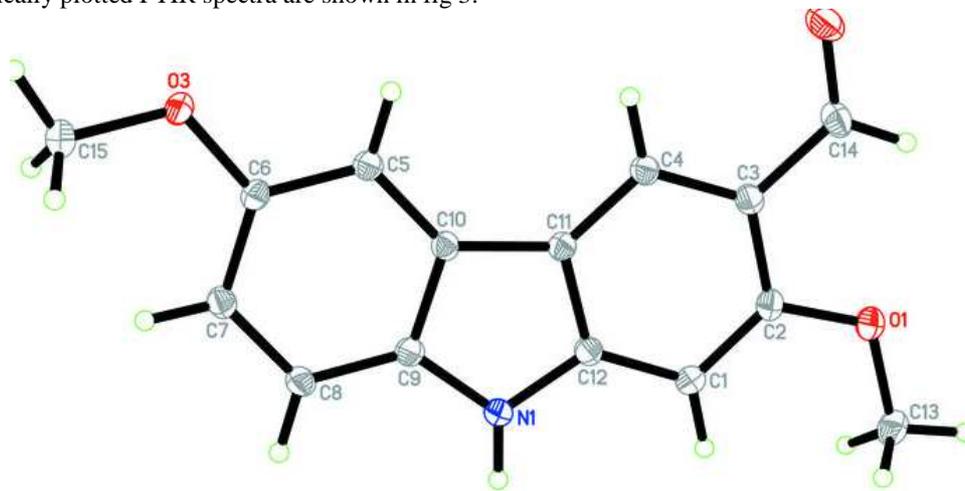


Fig 1. Molecular structure of Glycozolidal according to numbering scheme

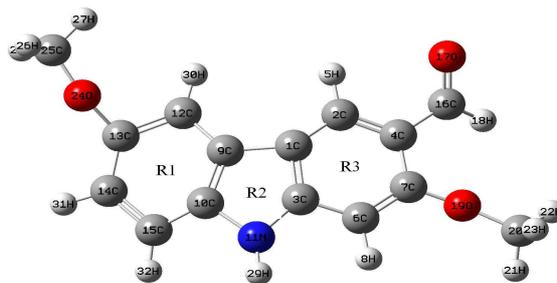


Fig 2. 3D Molecular structure of Glycozolidal as obtained by gaussview.

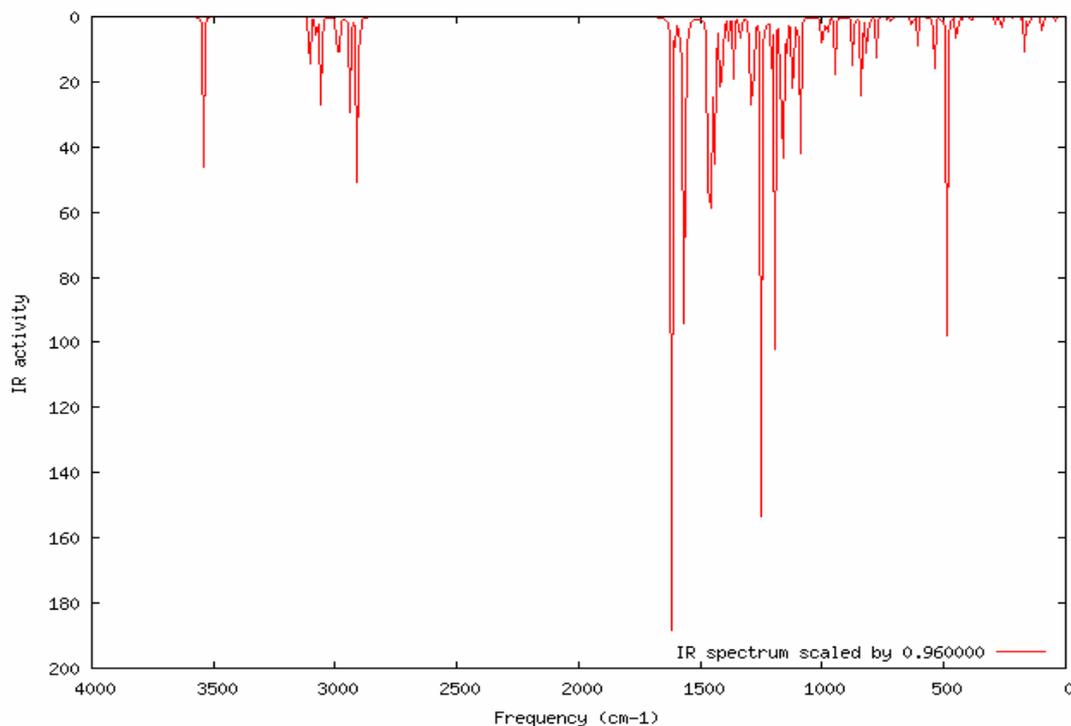


Fig 3. Theoretically plotted IR spectra for Glycozolidal

### 3. Computational Details

The entire calculations were performed on an AMD dual core/2.71 GHZ personal computer using Gaussian 03W [5] program package, invoking gradient geometry optimization [6]. Initial geometry was generated from standard geometrical parameters and was minimized without any constraint in the potential energy surface at B3LYP level, adopting the standard LanL2DZ basis set. The optimized structural parameters were used in the vibrational frequency calculations to characterize all stationary points as minima. We have utilized the gradient corrected density functional theory (DFT) [7] with the three-parameter hybrid functional (B3LYP) [8] for the exchange part and the Lee–Yang–Parr (LYP) correlation function [9] for the computation of molecular structure, vibrational frequencies, and energies of the optimized structures. Vibrational frequencies computed at DFT level have been adjudicated to be more reliable than those obtained by the computationally demanding Moller–Plesset perturbation methods. DFT offers electron correlation which is frequently comparable to second-order Moller–Plesset theory (MP2) [10,11]. Vibrational frequencies calculated at B3LYP/LanL2DZ level were scaled by a factor of 0.96 [12]. The calculated normal mode vibrational frequencies were analyzed in terms of the PED contributions by using the VEDA program [4].

## RESULTS AND DISCUSSION

### 4.1 Geometry Optimization.

The optimized structure parameters of glycozolidal calculated by DFT, B3LYP level with the LanL2DZ basis set are listed in Table 1; the atom numbering scheme is given in Fig. 1. Experimental values of bond lengths and angles of glycozolidal are taken from literature [3]. For example the optimized bond lengths of (C-C) in ring R3 falls in the range [1.3982-1.4346 Å], which are in good agreement with those of experimental bond lengths [1.3892-1.4637]; optimized bond lengths of (C-C) in the range [1.401-1.4198 Å] for B3LYP method which are in good agreement with the experimental bond lengths [1.3896-1.4013 Å]; the optimized bond length of (C-N) in ring R2 falls in the range [1.907-1.4127 Å] which are in good agreement with those in experimental x-ray data found in the range [1.3702-1.3927 Å]. The optimized bond lengths of (C-O) adjacent ring R1 & R2 are found to be in the range [1.3949-1.4564 Å], which are also in good agreement with experimental values fall in the range [1.3667-1.4347 Å]. The optimized bond length of (C=O) adjacent R3 is calculated as 1.2568 Å which is in very good agreement with the experimental value found to be 1.2225 Å.

Table 1: Optimized geometrical parameters of Glycozolidal at B3LYP/ LanL2DZ Level

S.No.	Parameter	DFT Method Bond lengths(Å)	X-ray-data	S.No.	Parameter	DFT Method Bond angles(deg)	X-ray-data
1	C4—C11	1.3982	1.3892	37	C12—C11—C10	106.9407	106.47
2	C11—C12	1.4346	1.4212	38	C11—C4—C3	120.2747	120.02
3	C10—C11	1.4585	1.4516	39	C11—C4—H4A	122.3262	120
4	C3—C4	1.4105	1.3995	40	C3—C4—H4A	117.3991	120
5	C4—H4A	1.0869	0.95	41	C1—C12—C11	122.4006	123.1
6	C1—C12	1.4073	1.3944	42	N1—C12—C11	108.4485	109.3
7	N1—C12	1.3907	1.3702	43	N1—C12—C1	129.151	127.59
8	C2—C3	1.4343	1.425	44	C4—C3—C2	119.5569	120.03
9	C3—C14	1.4754	1.4637	45	C4—C3—C14	119.6095	119.5
10	C1—C2	1.4052	1.389	46	C2—C3—C14	120.8336	120.45
11	C1—H1A	1.0845	0.95	47	C2—C1—C12	117.4124	117.29
12	O1—C2	1.3949	1.3667	48	C12—C1—H1A	120.8995	121.4
13	C9—C10	1.4234	1.4158	49	C2—C1—H1A	121.6882	121.4
14	C5—C10	1.4103	1.3962	50	C1—C2—C3	121.4827	121.15
15	N1—C9	1.4127	1.3927	51	O1—C2—C3	115.4094	115.86
16	C8—C9	1.4044	1.3896	52	O1—C2—C1	123.1079	122.99
17	N1—H1N1	1.0097	0.89	53	C9—C10—C11	106.7886	106.16
18	C5—C6	1.4063	1.3954	54	C5—C10—C11	133.0621	134.11
19	C5—H5A	1.085	0.95	55	C5—C10—C9	120.1493	119.72
20	C6—C7	1.4198	1.4013	56	N1—C9—C10	108.4475	109.1
21	O3—C6	1.4009	1.3887	57	C8—C9—C10	121.6305	121.59
22	C7—C8	1.401	1.3975	58	C8—C9—N1	129.9221	129.31
23	C7—H7A	1.0856	0.95	59	C12—N1—C9	109.3748	108.96
24	C8—H8A	1.0869	0.95	60	C12—N1—H1N1	125.5432	123.8
25	O2—C14	1.2568	1.2225	62	C9—N1—H1N1	125.082	127.2
26	C14—H14A	1.1006	0.95	63	C6—C5—C10	118.1705	118.43
27	O1—C13	1.4564	1.4347	64	C10—C5—H5A	120.2393	120.8
28	C13—H13A	1.0987	0.98	65	C6—C5—H5A	121.5902	120.8
29	C13—H13B	1.0915	0.98	66	C5—C6—C7	121.1685	121.67
30	C13—H13C	1.0987	0.98	67	O3—C6—C5	124.3296	115.45
31	O3—C15	1.4552	1.4337	68	O3—C6—C7	114.502	122.88
32	C15—H15A	1.0919	0.98	69	C8—C7—C6	120.9581	120.15
33	C15—H15B	1.0993	0.98	70	C6—C7—H7A	117.8853	119.9
34	C15—H15C	1.0993	0.98	71	C8—C7—H7A	121.1567	119.9
	Bond angles(deg)			72	C9—C8—C7	117.9232	118.4
35	C4—C11—C12	118.8728	118.4	73	C9—C8—H8A	121.7895	120.8
36	C4—C11—C10	134.1865	135.13	74	C7—C8—H8A	120.2873	120.8
75	O2—C14—C3	123.5689	124.07	116	C1—C2—C3—C4	-0.0009	-0.33
76	C3—C14—H14A	115.9111	118	117	O1—C2—C3—C4	180.0016	179.41
77	O2—C14—H14A	120.5201	118	118	C1—C2—C3—C14	180.0014	178.23
78	C2—O1—C13	119.2876	116.31	119	O1—C2—C3—C14	0.0039	-2.02
79	O1—C13—H13A	111.1083	109.5	120	C4—C3—C14—O2	-0.019	-3.35
80	O1—C13—H13B	105.2275	109.5	121	C4—C3—C14—H18	179.9812	NA
81	O1—C13—H13C	111.1061	109.5	122	C2—C3—C14—O2	179.9786	178.08
82	H13A—C13—H13B	109.7073	109.5	123	C2—C3—C14—H18	-0.0212	NA
83	H13A—C13—H13C	109.8867	109.5	124	C12—C1—C2—C3	0.0003	0.12
84	H13B—C13—H13C	109.7033	109.5	125	C12—C1—C2—O1	-180.0023	-179.61
85	C6—O3—C15	118.4123	116.91	126	H8—C1—C2—C3	-179.9968	NA
86	O3—C15—H15A	105.3794	109.5	127	H8—C1—C2—O1	0.0005	NA
87	O3—C15—H15B	111.2818	109.5	128	C13—O1—C2—C3	-179.9875	174.23
88	O3—C15—H15C	111.2786	109.5	129	C13—O1—C2—C1	0.0151	-6.03
89	H15A—C15—H15B	109.6306	109.5	130	N1—C9—C10—C11	0.0006	-0.55
90	H15A—C15—H15C	109.6268	109.5	131	C8—C9—C10—C11	179.9941	178.56
	H15B—C15—H15C	109.5574	109.5				
91	Dihedral angles			132	N1—C9—C10—C5	179.9954	-179.76
92	C3—C4—C11—C12	-0.0009	0.77	133	C8—C9—C10—C5	-0.0111	-0.65
93	C12—C11—C4—H5	179.9985	NA	134	C6—C5—C10—C11	-180.0093	179.98
94	C3—C4—C11—C10	179.995	-179.17	135	C11—C10—C5—H30	-0.003	NA
95	C10—C11—C4—H5	-0.0055	NA	136	C6—C5—C10—C9	-0.0025	-1.08
96	C4—C11—C12—C1	0.0003	-1.01	137	C9—C10—C5—H30	-179.9961	NA
97	C4—C11—C12—N1	179.9971	179.22	138	C12—N1—C9—C10	-0.0006	0.05
				139	C10—C9—N1—H29	179.9966	NA

98	C10—C11—C12—C1	-179.9966	178.95	140	C12—N1—C9—C8	-179.9934	-178.97
99	C10—C11—C12—N1	0.0001	-0.82	141	C8—C9—N1—H29	0.0038	NA
100	C9—C10—C11—C4	-179.9968	-179.22	142	C7—C8—C9—C10	0.0152	1.98
101	C5—C10—C11—C4	0.0094	-0.18	143	C10—C9—C8—H32	-179.9973	NA
102	C9—C10—C11—C12	-0.0004	0.83	144	C7—C8—C9—N1	180.0072	-179.11
103	C5—C10—C11—C12	-179.9942	179.87	145	N1—C9—C8—H32	-0.0053	NA
104	C2—C3—C4—C11	0.0012	-0.13	146	C10—C5—C6—C7	0.0114	1.47
105	C14—C3—C4—C11	179.9989	-178.71	147	C10—C5—C6—O3	180.0071	-178.94
106	H5—C4—C3—C2	-179.9983	NA	148	H30—C5—C6—C7	-179.995	NA
107	H5—C4—C3—C14	-0.0006	NA	149	H30—C5—C6—O3	0.0007	NA
108	C2—C1—C12—C11	0	0.56	150	C5—C6—C7—C8	-0.0073	-0.13
109	C11—C12—C1—H8	179.9971	NA	151	C5—C6—C7—H31	179.9976	NA
110	C2—C1—C12—N1	-179.9961	-179.72	152	O3—C6—C7—C8	179.9966	-179.69
111	N1—C12—C1—H8	0.0011	NA	153	O3—C6—C7—H31	0.0015	NA
112	C9—N1—C12—C11	0.0003	0.49	154	C15—O3—C6—C5	0.0233	-166.26
113	C11—C12—N1—H29	-179.9969	NA	155	C15—O3—C6—C7	180.0193	13.32
114	C9—N1—C12—C1	179.9967	-179.26	156	C6—C7—C8—C9	-0.0061	-1.58
115	C1—C12—N1—H29	-0.0004	NA	157	C6—C7—C8—H32	180.0062	NA
158	H31—C7—C8—C9	-180.0111	NA				
159	H31—C7—C8—H32	0.0012	NA				
160	C2—O1—C13—H21	61.3133	NA				
161	C2—O1—C13—H22	179.9794	NA				
162	C2—O1—C13—H23	-61.3604	NA				
163	C6—O3—C15—H26	-180.0052	NA				
164	C6—O3—C15—H27	-61.2498	NA				
165	C6—O3—C15—H28	61.2455	NA				

The other calculated bond lengths and bond angles also are in excellent agreement with the experimental values. Based on the above comparison although there some differences between the theoretical values and experimental values, the optimized structural parameters can well reproduce the experimental ones and they are the basis for thereafter discussion.

#### 4.2 Vibrational Assignments.

The title molecule has 32 atoms and 90 normal modes of fundamental vibrations. Detailed description of vibrational modes can be given by means of normal coordinate analysis. The vibrational assignments are achieved by considering the band positions and intensities with wave numbers and intensities from molecular modeling calculations at B3LYP/ LanL2DZ level. The experimental FT-IR spectrum of the title compound is not reported yet and the theoretical spectra are shown in Fig 2. Vibrational frequencies calculated at B3LYP/ LanL2DZ level were scaled by 0.96 [12]. The descriptions concerning the assignment have also been listed in Table 2. VEDA Program [4] was used for PED analysis and to assign the calculated harmonic frequencies. The harmonic vibrational frequencies calculated for glycozolidal at B3LYP level using LanL2DZ have been collected in Table 2. Several calculated thermodynamic parameters are presented in Table 3. The supplementary data related to all calculations are available from the corresponding author.

**4.2 (a) Carbonyl Absorption.** Carbonyl absorptions are sensitive and both the carbon and oxygen atoms of the carbonyl group move during the vibration and they have nearly equal amplitude. In the present study the C=O stretching vibration is obtained at 1619, 1603 and 1568  $\text{cm}^{-1}$  with potential energy distribution (PED) as 10%, 17% and 11% respectively. This stretching mode  $\nu(\text{C}=\text{O})$  is reported in the range 1620-1660  $\text{cm}^{-1}$  [13,14,15].

**4.2 b C-H Vibrations.** The hetero aromatic structure shows the presence of C-H stretching vibrations in the region 3000-3100  $\text{cm}^{-1}$  which is the characteristic region for the ready identification of the C-H stretching vibration [16]. In the present study the C-H stretching vibrations of the title compound are calculated at frequencies 3110, 3103, 3102, 3090 and 3076  $\text{cm}^{-1}$  with high PED values. The various bending vibrations assigned in this study are also supported by the literature [16].

**4.2c Methyl group vibrations.** The  $\text{CH}_3$  anti symmetric stretching vibrations are calculated at 3062, 3057, 2994 and 2985  $\text{cm}^{-1}$  with PED values 85%, 89%, 50% and 50% respectively., whereas  $\text{CH}_3$  symmetric vibrations are obtained

at 2911 and 2905  $\text{cm}^{-1}$ , with PED as 89% for both frequencies. These assignments are also supported by the literature [17]. In the present study various bending vibrations of CH<sub>3</sub> group are summarized in Table 2 and are also supported by the literature [17].

**Table 2. Vibrational wave numbers obtained for Glycozolidal at B3LYP/LanL2Z  
IR intensities and assignment with P.E.D. in square brackets**

S.No.	Wave No		IR Inten	Assignment [P.E.D.]
	Unsc	Scal		
	$\text{cm}^{-1}$		( $\text{Km}\cdot\text{mol}^{-1}$ )	
1	18	18	6	$\tau(\text{C10-C9-N1-C12})[20] + \tau(\text{C15-O3-C6-C5})[9]$
2	44	43	1	$\tau(\text{C11-C4-N1-C9})[21] + \tau(\text{C15-O3-C6-C5})[11]$
3	69	66	4	$\tau(\text{C13-O1-C2-C3})[16] + \tau(\text{C15-O3-C6-C5})[20]$
4	90	86	4	$\tau(\text{O2-C14-C3-C2})[12] + \tau(\text{C15-O3-C6-C5})[40]$
5	99	95	1	$\phi(\text{O3-C6-C7})[16]$
6	104	100	4	$\phi(\text{N1-C9-C8})[27] + \phi(\text{C14-C3-C4})[12]$
7	144	139	21	$\phi(\text{N1-C9-C8})[47] + \phi(\text{C14-C3-C4})[10]$
8	157	151	0	$\tau(\text{C8-C7-C13-C5})[21] + \tau(\text{O2-C14-C3-C2})[11] + \tau(\text{C2-C1-C4-N1})[16]$
9	174	167	1	$\tau(\text{O2-C14-C3-C2})[47] + \tau(\text{H14A-C14-C3-C2})[11]$
10	179	172	1	$\phi(\text{C13-O1-C2})[14] + \phi(\text{O1-C2-C1})[23]$
11	190	183	1	$\phi(\text{C14-C3-C4})[13] + \phi(\text{O1-C2-C1})[15] + \phi(\text{O3-C6-C7})[19]$
12	218	210	1	$\tau(\text{H13A-C13-O1-C2})[13] + \tau(\text{H13B-C13-O1-C2})[13] + \tau(\text{H13C-C13-O1-C2})[13]$
13	253	243	10	$\omega(\text{N1-C10-C8-C9})[12] + \tau(\text{H15A-C15-O3-C6})[14]$
14	272	261	3	$\phi(\text{C15-O3-C6})[27] + \phi(\text{C13-O1-C2})[13] + \phi(\text{C14-C3-C4})[10] + \phi(\text{O3-C6-C7})[12]$
15	300	288	1	$\tau(\text{C11-C12-N1-C9})[10] + \tau(\text{C2-C1-C12-N1})[28]$
16	372	357	2	$\tau(\text{C10-C5-C6-C7})[10]$
17	397	382	2	$\omega(\text{C4-C10-C12-C11})[23] + \omega(\text{C14-C2-C4-C20})[20] + \tau(\text{C10-C5-C6-C7})[10]$
18	408	392	1	$\omega(\text{O3-C5-C7-C6})[21] + \omega(\text{N1-C2-C4-C20})[20]$
19	425	408	1	$\phi(\text{C13-O1-C2})[18] + \phi(\text{C15-O3-C6})[16]$
20	462	443	5	$\omega(\text{C4-C10-C12-C11})[18] + \omega(\text{C1-N1-C11-C12})[20]$
21	467	449	6	$\omega(\text{O1-C3-C1-C2})[19]$
22	470	451	20	$\omega(\text{C4-C10-C12-C11})[11] + \tau(\text{C3-C4-C11-C10})[12]$
23	501	481	110	$\omega(\text{C4-C10-C12-C11})[21] + \tau(\text{C3-C4-C11-C10})[10]$
24	509	488	57	$\phi(\text{C15-O3-C6})[14]$
25	560	538	57	$\tau(\text{H29-N1-C12-C1})[89]$
26	627	602	9	$\omega(\text{O3-C5-C7-C6})[25]$
27	635	610	1	$\phi(\text{C8-C7-C6})[16] + \tau(\text{H7A-C7-C8-C9})[11]$
28	656	630	9	$\phi(\text{O2-C14-C3})[19] + \phi(\text{C1-C12-C11})[17]$
29	709	681	0	$\omega(\text{C1-N1-C11-C12})[10]$
30	730	701	4	$\tau(\text{C1-C2-C3-C4})[10]$
31	750	720	6	$\phi(\text{C12-N1-C9})[18]$
32	768	737	1	$\nu(\text{C2-O1})[14] + \phi(\text{C4-C11-C12})[15] + \tau(\text{C11-C12-N1-C9})[10]$
33	799	767	2	$\omega(\text{C4-C10-C12-C11})[15] + \tau(\text{C11-C12-N1-C9})[12]$
34	807	775	19	$\tau(\text{C11-C12-N1-C9})[12]$
35	849	815	53	$\tau(\text{H8A-C8-C7-C6})[43]$
36	860	826	7	$\phi(\text{C8-C7-C6})[16] + \tau(\text{H31-C7-C8-C9})[11]$
37	875	840	48	$\tau(\text{H1A-C1-C12-N1})[77]$
38	906	870	4	$\tau(\text{C10-C5-C6-C7})[14]$
39	908	872	37	$\tau(\text{H5A-C5-C6-C7})[34]$
40	980	941	7	$\tau(\text{H4A-C4-C11-C10})[70]$
41	985	946	0	$\tau(\text{H7A-C7-C8-C9})[36] + \tau(\text{H8A-C8-C7-C6})[12]$
42	985	947	31	$\tau(\text{H7A-C7-C8-C9})[40]$
43	1018	981	21	$\nu(\text{C15-O3})[60]$
44	1038	997	6	$\tau(\text{H4A-C4-C11-C10})[16] + \omega(\text{C14-C2-C4-C3})[10]$
45	1039	998	49	$\tau(\text{H14A-C14-C3-C2})[64] + \omega(\text{C14-C2-C4-C3})[10]$
46	1134	1092	101	$\nu(\text{C2-O1})[26] + \tau(\text{H13B-C11-O1-C2})[37]$
47	1149	1104	0	$\tau(\text{H15C-C15-O3-C6})[17] + \tau(\text{H13C-C13-O1-C2})[18]$
48	1151	1106	0	$\tau(\text{H15A-C15-O3-C6})[38] + \tau(\text{H15B-C15-O3-C6})[17]$
49	1160	1119	145	$\phi(\text{H7A-C7-C6})[13] + \phi(\text{H8A-C8-C9})[15]$
50	1187	1141	2	$\tau(\text{H15B-C15-O3-C6})[19] + \tau(\text{H15C-C15-O3-C6})[19]$
51	1194	1147	10	$\nu(\text{C13-O1})[17] + \tau(\text{H15A-C15-O3-C6})[16]$
52	1208	1160	87	$\nu(\text{C15-O3})[17] + \phi(\text{H13C-C13-O1})[13]$
53	1215	1166	133	$\nu(\text{C-C})\text{R3Symm}[14]$
54	1242	1195	109	$\phi(\text{H1N1-N1-C12})[28]$
55	1259	1211	19	$\omega(\text{H1N1-N1-C12})[28]$
56	1283	1232	13	$\nu(\text{C9-N1})[14]$
57	1301	1250	194	$\nu(\text{C-C})\text{R3}[10]$
58	1340	1287	143	$\nu(\text{C-C})\text{R1}[10]$

59	1348	1294	52	$\nu(\text{C12-N1})[16]$
60	1391	1336	29	$\phi(\text{H14A-C14-O2})[22]+\nu(\text{C-C})\text{R3}[22]$
61	1420	1363	22	$\phi(\text{H14A-C14-O2})[30]$
62	1443	1385	13	$\phi(\text{H14A-C14-O2})[24]$
63	1472	1414	122	$\phi(\text{H15A-C15-H15C})\text{boat}[16]$
64	1480	1421	22	$\phi(\text{H13A-C13-H13C})\text{boat}[16]$
65	1495	1436	10	$\phi(\text{H15A-C15-H15C})[15]+\phi(\text{H13B-C13-H13C})[13]+\phi(\text{H13A-C13-H13B})[10]$
66	1501	1441	91	$\nu(\text{C-C})\text{R1}[11]$
67	1512	1452	13	$\phi(\text{H15A-C15-H15C})\text{rock}[39]$
68	1515	1454	14	$\phi(\text{H13A-C13-H13B})[39]$
69	1516	1456	156	$\phi(\text{H13A-C13-H13B})[39]$
70	1520	1459	17	$\phi(\text{H15A-C15-H15C})[40]+\nu(\text{C-C})\text{R3}[11]$
71	1524	1463	60	$\phi(\text{H13C-C13-H21})[39]+\phi(\text{H15A-C15-H15C})[13]$
72	1529	1468	71	$\nu(\text{C-C})\text{R3}[11]$
73	1615	1551	19	$\nu(\text{C-C})\text{R1}[21]+\nu(\text{C14=O2})[11]$
74	1632	1568	407	$\nu(\text{C14=O2})[11]$
75	1637	1573	94	$\nu(\text{C-C})\text{R3}[25]$
76	1668	1603	7	$\nu(\text{C14=O2})[17]+\nu(\text{C-C})\text{R2}[10]$
77	1686	1619	189	$\nu(\text{C14=O2})[10]+\nu(\text{C-C})\text{R1}[13]$
78	3024	2905	52	$\nu(\text{C15-H3})\text{asym}[45]+\nu(\text{C13-H3})\text{symm}[44]$
79	3029	2911	64	$\nu(\text{C13-H3})\text{asym}[45]+\nu(\text{C13-H3})\text{symm}[44]$
80	3062	2940	70	$\nu(\text{C14-H14A})[100]$
81	3109	2985	53	$\nu(\text{C15-H3})[50]$
82	3119	2994	49	$\nu(\text{C13-H3})\text{symm}[50]$
83	3183	3057	35	$\nu(\text{C15-H3})[89]$
84	3190	3062	25	$\nu(\text{C13-H3})\text{symm}[89]$
85	3204	3076	12	$\nu(\text{C8-H8A})[89]+\nu(\text{C7-H7A})[10]$
86	3218	3090	1	$\nu(\text{C4-H5A})\text{asym}[99]$
87	3231	3102	16	$\nu(\text{C5-H5A})\text{asym}[72]$
88	3232	3103	1	$\nu(\text{C1-H1A})\text{asym}[74]$
89	3238	3110	8	$\nu(\text{C7-H7A})\text{asym}[88]+\nu(\text{C8-H8A})\text{asym}[10]$
90	3689	3542	65	$\nu(\text{N1-H1N1})[100]$

Note: Abbreviations used here have following meaning.  $\nu$ : stretching;  $\nu\text{symm}$ : symmetric stretching;  $\nu\text{asym}$ : asymmetric stretching;  $\phi$ : in-plane bending;  $\omega$ : out-of-plane bending;  $\tau$ : torsion; R: Ring; adj: adjacent.

**4.2d (C-C) Ring Vibrations.** The C–C aromatic stretch known as semi-circle stretching are calculated at frequencies 1441, 1336, 1287, 1250 and 1166  $\text{cm}^{-1}$  with low PED values as shown in Table 2. In literature [18,19] the  $\nu(\text{C-C})$  in plane stretching mode is reported at frequency 1327  $\text{cm}^{-1}$ . The out of plane vibrations according to Whiffen [20] are well known although, it is more difficult to find force field for these vibrations.

**4.2e (C–N) Vibrations.** The identification of C–N vibrations is a difficult task, since the mixing of vibrations is possible in this region. In this study the C–N stretching vibrations are calculated at frequencies 1294 and 1232  $\text{cm}^{-1}$  with PED values as 16% and 14% respectively. The various bending and torsional vibrations assigned in this study are also supported by the literature [21].

**4.2f (C–O) Vibrations.** In this study the C–O stretching vibrations are calculated at 1160, 1147, 1092 and 981  $\text{cm}^{-1}$  with PED as 17%, 17%, 26% and 60% respectively, these stretching as well as various bending vibrations are well supported by the literature [22].

**4.2g (N–H) Vibrations.** The stretching vibration of  $\nu(\text{N-H})$  is calculated at 3542  $\text{cm}^{-1}$  with 100% PED. Some bending vibrations are calculated and the values are supported by the literature [23].

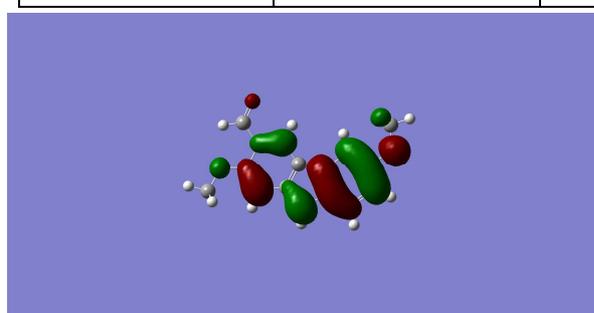
**4.2h Other Molecular and Electronic properties.** The frontier orbitals, HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) determine the way a molecule interacts with other species. The frontier orbital gap helps characterize the chemical reactivity and kinetic stability of the molecule. A molecule with a small frontier orbital gap is more polarizable and is generally associated with a high chemical reactivity, low kinetic stability and is also termed as soft molecule [24]. The frontier orbital gap in case of Glycozolidal is found to be 3.63 eV, which suggests probably the high kinetic stability, low polarizability. The HOMO is the orbital that primarily acts as an electron donor and the LUMO is the orbital that largely acts as the electron acceptor. The 3D plots of the frontier orbitals HOMO and LUMO and electron density (ED) for the title molecule are shown in Fig 4, Fig. 5 and Fig. 6. The dipole moment in a molecule is an important property that is

mainly used to study the intermolecular interactions involving the non bonded type dipole-dipole interactions, because higher the dipole moment, stronger will be the intermolecular interactions. For the studied molecule the dipole moment is calculated as 5.6353 Debye.

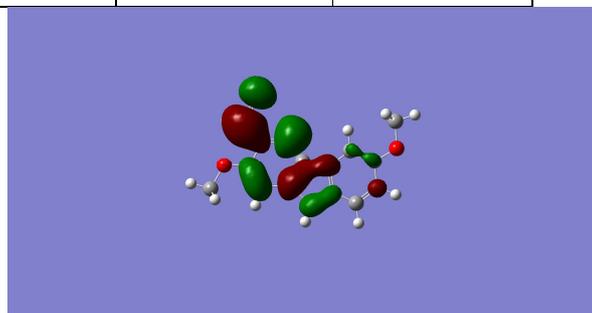
Several other thermodynamic parameters calculated at B3LYP/ LanL2DZ level are presented in Table 3. In this study total energy of the title compound is calculated as -859.22 KCal/Mol, while zero point energy is obtained as 153.58 KCal/Mol. Values of rotational constants are found to be 0.78913, 0.18998 and 0.15577 GHz. The total entropy is calculated as 127.517 Cal/Mol-K comprising the vibrational part as maximum.

**Table 3. Theoretically computed zero-point vibrational energy, rotational constants, entropies and dipole moment for Glycozolidal.**

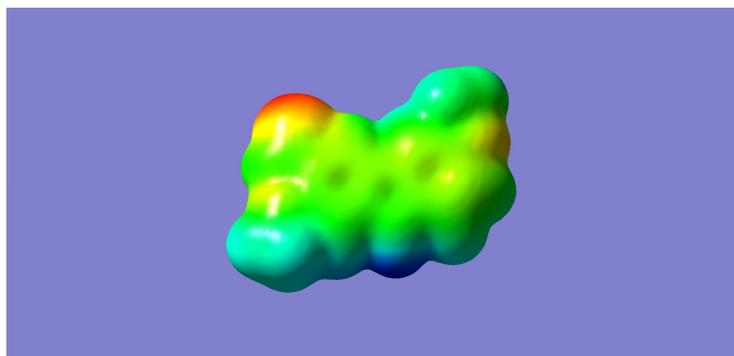
	Entropy (S) Cal/Mol-Kel	Rotational const(GHZ)	Total energy (kcal/mol)	Dipole mom(Debye)	Zero pt Vib Energy (Kcal/Mol)
Total	127.517	0.78913			
Electronic	0.000	0.18998			
Translational	42.509	0.15577	-859.22	5.6353	153.57925
Rotational	33.900				
Vibrational	51.108				



**Fig 4. HOMO of Glycozolidal**



**Fig 5. LUMO of Glycozolidal**



**Fig 6. Total density of Glycozolidal**

## CONCLUSION

The equilibrium geometries and harmonic frequencies of glycozolidal, reported to be bioactive molecule, were determined and analyzed at DFT B3LYP/LanL2DZ level of theory. The vibrational frequency calculation proved that the structure is stable (no imaginary frequencies). Although neither the FTIR nor Raman spectra of the title molecule, are reported, still the theoretical study of vibrational dynamics, geometry optimization, electronic properties and thermodynamical parameters are of great importance for the better insight of the title compound. With the continuing need for novel structures and the difficulty of gaining access to large tracts of biodiversity in

habitats, combinatorial chemistry blended with modern quantum chemical methods can prove to be extremely useful for the researchers.

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