Prediction of vibrational spectroscopic characteristics of bioactive natural product using density functional theory

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Abstract. The present study discusses the applicability of density functional theory to investigate the vibrational spectroscopy of some bioactive natural products implementing variety of functional-basis set combination to find out suitable theoretical model. The DFT at B3LYP/6-31+G (d,p) and at higher level functional-basis set combination have been obtained to be feasible for this purpose. The IR & Raman active vibrations at the normal modes have been obtained by the theoretical computation in the selected natural product namely Isodihydroaminocadambine. The vibrations in the various domains have been ascertained due to C-H stretching, C-H in plane bending, C–H out of plane bending, C–C stretching and other low domain frequencies calculated through the said theoretical approach. The theoretical IR spectra exhibit at most intensity at 388 cm⁻¹. The strongest Raman activity has been observed at 3202 cm⁻¹ which is the characteristics of this molecule. The spectroscopic characteristics reported in the present study may be applicable for characterizing the title molecule for exploring its different applications.

1. Introduction
Bioactive natural products have been promising materials since the ancient time and been emerged as an area of research because of its multifunctional applications involve no toll and drudge for their synthesis and having exquisite biophysical properties. Isodihydroaminocadambine is also a naturally occurring compound detached from the fruits of Anthocephalus cadamba plant possessing activity against the lung Cancer Cell Line H1299 [1-2], however the physical principle of its bioactivity to be reported yet. The computational study on such bioactive natural product has already accomplished a new aspect in the field of drug development and the same is also needed in case of selected compound in order to elaborate the physical principle of its bioactivity and to explore its application as a drug agent. The selected molecule has been taken up for the computational study on spectroscopic characteristics like IR active vibrations & Raman activity. The computational study has been performed using density functional theory (DFT) with B3LYP functional and 6-31+G(d,p) basis set because of its substantiated popularity in the recent reports [3-9]. The specific short-range (Eₐ) and long range (Eₐ') part of the exchange interaction
Eₓ=−(1/2) Σₐ ∫ ρₐ ⁴/₃ Kₐ d³r, is integrated by modifying the common exchange functional form as expressed by equation 1 and 2 respectively [10-11].
\[ E^{\text{fr}}_x = -\left(\frac{1}{2}\right) \sum_{\sigma} \rho^{4/3} K_\sigma \times \left(1 - \frac{8}{3} a_\sigma \sqrt{\pi} \text{erf} \left(\frac{1}{2a_\sigma}\right) + 2a_\sigma (b_\sigma - c_\sigma)\right) d^3r \]  

Where \( a_\sigma, b_\sigma \) and \( c_\sigma \) are:
\[
a_\sigma = \frac{\mu k_\sigma^2}{6\sqrt{\pi \rho_0^3}},
\]
\[
b_\sigma = \exp \left(\frac{1}{4a_\sigma}\right) - 1,
\]
\[
c_\sigma = 2a_\sigma^2 b_\sigma + \frac{1}{2}
\]
\[ E^{\text{fr}}_x = -\frac{1}{2} \sum_{\alpha \beta} \sum_{i \sigma} \sum_{j \sigma} \int \int \psi_i^\alpha(\mathbf{r}_1) \psi_j^\beta(\mathbf{r}_1) \times \text{erf} \left(\frac{\omega_{ij}}{r_{ij2}}\right) \psi_i^\alpha(\mathbf{r}_2) \psi_j^\beta(\mathbf{r}_2) d^4r_1 d^4r_2 
\] 

Where, \( \psi_i^\alpha \) represents the \( i \)th \( \sigma \)-spin molecular orbital and the used parameter \( \mu \) ascertains the balance of DFT to HF exchange at intermediate \( r_{ij2} \).

2. Computational Methods

2.1 Density Functional Theory Approach

In this work, the geometry optimization and frequency calculation were performed at DFT-B3LYP/6-31+G (d,p) level of theory as per reported method [12-13]. DFT provides a better settlement between computational cost and accuracy too for such type of molecules. The evaluation of IR and Raman activity were carried out using normal mode analysis of the calculated frequencies at the same theoretical level and its frequency calculation at the same level of theory were performed to ascertain the existence of true minimum at the potential surface implemented in GAUSSIAN 09 program package [14].

3. Results

3.1 Geometry Optimization

The optimized geometry of the selected molecule having molecular formula C_{26}H_{33}N_{3}O_{7} consisting of 69 atoms containing nonlinearity due to asymmetric atomic charge distribution obtained using said theoretical model has been depicted in figure 1.

Figure 1. Optimized Geometry of Isodihydroaminocadambine
Blue spheres indicate N-atoms, Red spheres to O-atoms, Black spheres to C-atoms and white spheres to H-atoms.

3.2 Vibrational Analysis

Vibrational spectroscopy furnishes important information related to the structure and properties of molecules. The normal mode analysis of IR active vibrations is specific feature of theoretical computation. The normal mode analysis of the vibrational frequency demonstrates 201 active fundamental modes of vibration which are aligned with the well-known formula of maximum (3N-6) numbers of such modes of vibrations in a nonlinear molecule having N atoms [15]. There is no imaginary frequency in these active modes showing the existence of true minimum at potential surface. The calculated vibrational frequencies of these fundamental modes are designated through gauss-view program [16]. The calculated frequency of each fundamental mode has been scaled with a factor of 0.9648 because the hybrid functional B3LYP in DFT approach tends to overestimate the fundamental modes as prescribed by Merrick et al [17]. The calculated and scaled frequencies of IR active mode of vibrations and its Raman activity have been shown in Table 1 and theoretical IR Spectra have been depicted in figure 2.

![Figure 2. IR spectra of Isodihydroaminocadambine](image_url)

| Mode of Vibrations | Calculated freq. (cm⁻¹) | Scaled freq. (cm⁻¹) | Intensity (IR) | Raman Activity (Å²/AMU) | P-Depolar | U-Depolar | Vibration Descriptions |
|-------------------|-------------------------|---------------------|----------------|-------------------------|------------|------------|-----------------------|
| 1                 | 18                      | 17                  | 0.1832         | 1.6453                  | 0.7103     | 0.8306     | τ₁(C₃₂–H₆₁)          |
| 2                 | 22                      | 21                  | 0.1113         | 3.1715                  | 0.7482     | 0.8560     | σ(H₆₀–C₃₂–H₆₁)       |
| 3                 | 32                      | 31                  | 0.2106         | 2.8025                  | 0.7454     | 0.8542     | σ(H₆₀–C₃₂–H₆₁)       |
| 4                 | 42                      | 40                  | 0.3097         | 2.1372                  | 0.7478     | 0.8557     | τ₀(C₃₂–H₆₁)          |
| 5                 | 53                      | 52                  | 0.2188         | 1.5903                  | 0.7469     | 0.8551     | ρ(H₆–C₄–H₅₃)          |
| Mode of Vibration | Calculated freq. (cm⁻¹) | Scaled freq. (cm⁻¹) | Intensity (IR) | Raman Activity (Å²/AMU) | P-Depolar | U-Depolar | Vibration Descriptions |
|-------------------|-------------------------|--------------------|---------------|-------------------------|-----------|-----------|-----------------------|
| 6                 | 65                      | 62                 | 0.7580        | 5.0331                  | 0.7499    | 0.8571    | R[τ₀(C10–H15)]        |
| 7                 | 66                      | 64                 | 0.2353        | 0.6538                  | 0.709     | 0.8297    | R{τ₀(C9–H14)} + σ(H23–C22–H55) |
| 8                 | 82                      | 79                 | 3.7751        | 0.4041                  | 0.598     | 0.7484    | τ₀{(O45–H46)+(O47–H52)} |
| 9                 | 95                      | 92                 | 0.3288        | 0.9249                  | 0.7487    | 0.8563    | τ₀(C31–H59) + τ₀(C32–H61) |
| 10                | 111                     | 107                | 2.0556        | 0.2756                  | 0.75      | 0.8571    | ρ(C44–H63–H64) |
| 11                | 126                     | 121                | 9.8791        | 0.1180                  | 0.6877    | 0.8150    | ρ(C1–H5–H54) + τ₀(N66–H67–H68) |
| 12                | 132                     | 127                | 0.8724        | 1.8277                  | 0.7331    | 0.8460    | ρ(C32–H60) + τ₀(C9–H14) |
| 13                | 145                     | 140                | 0.5725        | 0.5691                  | 0.4343    | 0.6056    | σ(H23–C22–H55) + τ₀(N66–H67–H68) |
| 14                | 149                     | 143                | 2.0378        | 0.6790                  | 0.6582    | 0.7939    | ρ(H63–C44–H64) + τ₀(O45–H46) |
| 15                | 154                     | 149                | 0.4642        | 1.5398                  | 0.2295    | 0.3733    | ρ(H63–C44–H64) + τ₀(O45–H46) |
| 16                | 164                     | 159                | 0.4747        | 0.5624                  | 0.5512    | 0.7107    | σ(H60–C32–H61) |
| 17                | 180                     | 174                | 0.1541        | 0.4402                  | 0.1207    | 0.2154    | ρ(C32–H60) + τ₀(C32–H60) |
| 18                | 189                     | 182                | 0.8417        | 0.4639                  | 0.7491    | 0.8566    | ρ(H63–C44–H64) + τ₀(O45–H46) |
| 19                | 206                     | 199                | 0.4411        | 1.1428                  | 0.1898    | 0.3190    | ρ(H32–C22–H55) + τ₀(O45–H46) |
| 20                | 212                     | 204                | 1.9876        | 0.9900                  | 0.5616    | 0.7193    | ρ(H6–C4–H53) + τ₀(C32–H60) |
| 21                | 225                     | 217                | 34.5709       | 2.1777                  | 0.5067    | 0.6726    | τ₀(O47–H52) + τ₀(O49–H50) |
| 22                | 246                     | 237                | 8.5742        | 0.2027                  | 0.5760    | 0.1089    | ρ(C1–H5–H54) |
| 23                | 248                     | 239                | 2.6561        | 1.4712                  | 0.3707    | 0.5409    | ρ(N66–H67–H68) |
| 24                | 261                     | 252                | 4.7025        | 0.9473                  | 0.4164    | 0.5880    | ρ(N66–H67–H68) + τ₀(O49–H50) |
| 25                | 267                     | 257                | 6.6369        | 1.2363                  | 0.4244    | 0.5959    | ρ(N66–H67–H68) |
| 26                | 273                     | 263                | 35.1694       | 0.3306                  | 0.5075    | 0.6733    | τ₀(O47–H52) + τ₀(O48–H51) |
| 27                | 280                     | 270                | 11.2447       | 1.6298                  | 0.2432    | 0.3913    | ρ(N66–H67–H68) + τ₀(O49–H50) |
| 28                | 296                     | 285                | 1.5669        | 0.8864                  | 0.2753    | 0.4318    | τ₀(C24–H72) + τ₀(C32–H60) |
| 29                | 302                     | 292                | 2.3954        | 0.2705                  | 0.6225    | 0.7673    | ρ(H63–C44–H64) + τ₀(O49–H50) |
| 30                | 311                     | 300                | 2.4523        | 0.3367                  | 0.1996    | 0.3328    | ρ(C4–H6–H53) |
| Mode of Vibration | Calculated freq. (cm⁻¹) | Scaled freq. (cm⁻¹) | Intensity (IR) | Raman Activity (Å³/AMU) | P-Depolar | U-Depolar | Vibration Descriptions |
|------------------|-------------------------|--------------------|---------------|-------------------------|-----------|-----------|-----------------------|
| 31               | 316                     | 305                | 1.4093        | 5.2421                  | 0.1146    | 0.2056    | ρ(C1–H54–H5)+\(τ_i(C45–H46)\) |
| 32               | 342                     | 330                | 8.1085        | 1.3285                  | 0.4848    | 0.6531    | ρ(C32–H60–H61)+\(τ_0(C37–H62)\) |
| 33               | 351                     | 339                | 7.1446        | 3.0980                  | 0.5306    | 0.6933    | ρ(C4–H6–H53)          |
| 34               | 368                     | 355                | 4.2685        | 0.4866                  | 0.3967    | 0.5681    | R[τ_0(C8–H13)+(C11–H16)]+ρ(C4–H6–H53) |
| 35               | 388                     | 374                | 98.6830       | 1.5197                  | 0.3547    | 0.5237    | τ_0(O47–H52)+τ_0(O48–H51) |
| 36               | 396                     | 382                | 38.0034       | 2.9700                  | 0.5138    | 0.6788    | ρ(H60–C32–H61)+τ_0(O47–H52) |
| 37               | 418                     | 403                | 12.3699       | 2.3421                  | 0.7149    | 0.8338    | ρ(H60–C32–H61)+τ_0(O48–H51) |
| 38               | 421                     | 407                | 8.9962        | 2.4262                  | 0.3855    | 0.5565    | τ_0(O48–H51)+τ_0(O45–H54) |
| 39               | 429                     | 414                | 15.4568       | 1.8239                  | 0.4204    | 0.5919    | ρ(H60–C32–H61)+τ_0(O45–H54) |
| 40               | 442                     | 427                | 9.0561        | 1.5008                  | 0.5786    | 0.7330    | R[τ_0(C8–H13)+(C11–H16)]+τ_0(O49–H50) |
| 41               | 447                     | 431                | 51.6593       | 1.1838                  | 0.4441    | 0.6150    | R[τ_0(C8–H13)+(C11–H16)]+τ_0(C44–H63–H64) |
| 42               | 450                     | 435                | 79.2946       | 2.4151                  | 0.6859    | 0.8137    | τ_0(O49–H50)+τ_0(O45–H54) |
| 43               | 457                     | 440                | 67.7489       | 0.7589                  | 0.6019    | 0.7515    | τ_0(O45–H54)+τ_0(C22–H23–H55) |
| 44               | 486                     | 469                | 40.7244       | 1.3372                  | 0.6428    | 0.7826    | ρ(C22–H23–H55)+τ_0(C22–H23–H55) |
| 45               | 497                     | 480                | 1.1699        | 2.1371                  | 0.4226    | 0.5941    | ρ(C22–H23–H55)+τ_0(C32–H60–H61) |
| 46               | 504                     | 486                | 3.9192        | 4.2256                  | 0.2447    | 0.3931    | ρ(C32–H60–H61)+τ_0(C44–H63–H64) |
| 47               | 507                     | 490                | 4.4214        | 0.9624                  | 0.5663    | 0.7231    | ρ(C44–H63–H64)+τ_0(O45–H54) |
| 48               | 524                     | 506                | 0.2301        | 1.6606                  | 0.3657    | 0.5356    | τ_0(C32–H60–H61)+τ_0(C25–H57) |
| 49               | 542                     | 523                | 6.6012        | 4.9660                  | 0.2772    | 0.4341    | ρ(C4–H6–H53)+τ_0(C22–H23–H55) |
| 50               | 547                     | 528                | 18.6677       | 3.2643                  | 0.136    | 0.2395    | ρ(H60–C32–H61)+τ_0(C44–H63)+τ_0{(C9–H14)+(C10–H15)}+τ_0(N17–H18) |
| 51               | 588                     | 568                | 22.9775       | 5.1603                  | 0.6343    | 0.7762    | τ_0{(C9–H14)+(C10–H15)}+τ_0(N17–H18) |
| 52               | 572                     | 552                | 6.3012        | 1.3600                  | 0.6687    | 0.8015    | ρ(C44–H63–H64)+τ_0(C35–H39) |
| 53               | 582                     | 561                | 0.3656        | 3.0712                  | 0.6293    | 0.7725    | R[τ_0(C10–H15)+τ_0(C9–H14)] |
| 54               | 601                     | 580                | 17.7454       | 2.7017                  | 0.3846    | 0.5555    | R[τ_0(C10–H15)]+τ_0(N17–H18) |
| Mode of Vibrations | Calculated freq. (cm\(^{-1}\)) | Scaled freq. (cm\(^{-1}\)) | Intensity (IR) | Raman Activity (Å/AMU) | P-Depolar | U-Depolar | Vibrations Descriptions |
|-------------------|-------------------------------|-----------------------------|----------------|------------------------|------------|------------|------------------------|
| 55                | 609                           | 587                         | 12.6583        | 1.5897                 | 0.6515     | 0.7890     | \(\tau_0(\text{N17–H18})\) |
| 56                | 618                           | 596                         | 2.4822         | 2.1963                 | 0.1922     | 0.3224     | \(R[\tau_0(\text{C9–H14})+\tau_0(\text{C8–H13})]\) |
| 57                | 644                           | 622                         | 16.5512        | 4.8876                 | 0.3228     | 0.4880     | \(\tau_0(\text{C31–H59})+\rho(\text{C32–H60–H61})\) |
| 58                | 651                           | 628                         | 1.9635         | 0.4059                 | 0.7484     | 0.8561     | \(\tau_0(\text{O47–H52})+\tau_i(\text{(O48–H51)}+\text{(O49–H50)})\) |
| 59                | 653                           | 630                         | 20.7961        | 1.6630                 | 0.5337     | 0.6960     | \(\tau_0(\text{C31–H59})+\rho(\text{C32–H60–H61})\) |
| 60                | 666                           | 642                         | 14.2758        | 2.7843                 | 0.4563     | 0.6266     | \(\tau_0(\text{C24–H27})+\tau_0(\text{C26–H58})\) |
| 61                | 678                           | 654                         | 15.9305        | 0.5863                 | 0.5568     | 0.7154     | \(\tau_0(\text{N17–H18})+\tau_0(\text{C26–H58})\) |
| 62                | 722                           | 697                         | 55.5437        | 1.2799                 | 0.7498     | 0.8570     | \(\rho(\text{C44–H63–H64})+\tau_0(\text{C36–H42})\) |
| 63                | 730                           | 705                         | 0.4468         | 17.8080                | 0.1221     | 0.2176     | \(\rho(\text{C44–H63–H64})+\tau_0(\text{C36–H42})\) |
| 64                | 737                           | 711                         | 32.0579        | 1.6497                 | 0.6485     | 0.7868     | \(\rho(\text{N66–H67–H68})\) |
| 65                | 751                           | 725                         | 57.5661        | 3.5915                 | 0.7071     | 0.8284     | \(\rho(\text{N66–H67–H68})\) |
| 66                | 762                           | 735                         | 9.1013         | 0.4558                 | 0.3977     | 0.5690     | \(\rho(\text{N66–H67–H68})\) |
| 67                | 774                           | 747                         | 12.5089        | 2.3803                 | 0.3372     | 0.5044     | \(\rho(\text{N66–H67–H68})\) |
| 68                | 778                           | 751                         | 26.0988        | 1.5219                 | 0.196      | 0.3278     | \(\rho(\text{C4–H6–H53})\) |
| 69                | 800                           | 772                         | 3.2994         | 20.7955                | 0.0592     | 0.1117     | \(\rho(\text{C4–H6–H53})\) |
| 70                | 824                           | 795                         | 134.2130       | 5.4971                 | 0.1257     | 0.2234     | \(\tau_0(\text{C35–H39})+\tau_0(\text{(O49–H50)}+\sigma(\text{H67–N66–H68})\) |
| 71                | 838                           | 809                         | 43.4364        | 1.4993                 | 0.2771     | 0.4340     | \(\sigma(\text{H67–N66–H68})\) |
| 72                | 857                           | 826                         | 1.1202         | 1.2719                 | 0.7446     | 0.8536     | \(\sigma(\text{H67–N66–H68})\) |
| 73                | 868                           | 838                         | 64.4036        | 2.2751                 | 0.0886     | 0.1628     | \(\sigma(\text{H67–N66–H68})\) |
| 74                | 876                           | 845                         | 17.3062        | 7.6076                 | 0.124      | 0.2206     | \(\sigma(\text{H67–N66–H68})\) |
| Mode of Vibrations | Calculated freq. (cm\(^{-1}\)) | Scaled freq. (cm\(^{-1}\)) | Intensity (IR) | Raman Activity (Å\(^5\)/AMU) | P-Depolar | U-Depolar | Vibration Descriptions |
|-------------------|-----------------------------|-----------------------------|----------------|-----------------------------|-----------|-----------|------------------------|
| 75                | 878                         | 847                         | 10.3424        | 2.2184                     | 0.3681    | 0.5381    | \(\tau_i(C38–H41)+\tau_0(C35–H39)\) |
| 76                | 887                         | 856                         | 2.8326         | 11.8273                    | 0.0915    | 0.1676    | \(R[\tau_i{(C11–H16)+(C9–H14)}]+\tau_0(N17–H18)\) |
| 77                | 895                         | 863                         | 25.4855        | 13.9783                    | 0.2866    | 0.4455    | \(\tau_i(C24–H27)+\tau_0(C36–H42)\) |
| 78                | 898                         | 866                         | 9.8310         | 8.5848                     | 0.2006    | 0.3342    | \(\rho(C4–H53–H6)+\tau_0(C37–H62)\) |
| 79                | 901                         | 869                         | 7.2832         | 2.0596                     | 0.4012    | 0.5726    | \(\rho(H60–C32–H61)\) |
| 80                | 925                         | 893                         | 3.6844         | 5.4710                     | 0.2894    | 0.4489    | \(R[\tau_i{(C8–H13)+(C11–H16)}]+\tau_0{(C9–H14)+(C10–H15)}\) |
| 81                | 934                         | 901                         | 4.3966         | 2.8413                     | 0.2954    | 0.4560    | \(R[\tau_i{(C8–H13)+(C11–H16)}]+\tau_0{(C9–H14)+(C10–H15)}\) |
| 82                | 934                         | 901                         | 7.9003         | 5.3655                     | 0.2414    | 0.3889    | \(R[\tau_i{(C8–H13)})+(C9–H14)\] \(\tau_0{(C1–H5)}\) |
| 83                | 949                         | 916                         | 11.5471        | 4.7534                     | 0.5723    | 0.7280    | \(\sigma(H6–N66–H68)\) |
| 84                | 962                         | 928                         | 163.5460       | 0.9636                     | 0.2258    | 0.3685    | \(\sigma(H60–C32–H61)\) |
| 85                | 972                         | 938                         | 10.3995        | 2.7613                     | 0.5957    | 0.7466    | \(\sigma(H60–C32–H61)\) |
| 86                | 972                         | 938                         | 0.1793         | 0.2238                     | 0.4067    | 0.5782    | \(\sigma(H60–C32–H61)\) |
| 87                | 979                         | 945                         | 15.9564        | 2.9675                     | 0.2376    | 0.3840    | \(\tau_0{(C1–H5)}+\tau_0{(C9–H14)+(C10–H15)}\) |
| 88                | 986                         | 951                         | 19.6876        | 2.6321                     | 0.7195    | 0.8369    | \(\rho(C44–H64–H63)\) |
| 89                | 1002                        | 967                         | 22.4028        | 3.7243                     | 0.5262    | 0.6896    | \(\sigma(H60–C32–H61)\) |
| 90                | 1006                        | 971                         | 27.5385        | 6.0052                     | 0.3129    | 0.4767    | \(\sigma(H60–C32–H61)\) |
| 91                | 1023                        | 987                         | 19.9918        | 4.4273                     | 0.5319    | 0.6944    | \(\tau_0{(C1–H5)}+\tau_0{(C9–H14)+(C10–H15)}\) |
| 92                | 1029                        | 992                         | 55.1423        | 21.0873                    | 0.2969    | 0.4578    | \(\sigma(H60–C32–H61)\) |
| 93                | 1032                        | 995                         | 71.3517        | 17.3046                    | 0.0309    | 0.0600    | \(R[\tau_i{(C9–H14)+(C10–H15)}]+\tau_0{(C31–H59)}\) |
| 94                | 1034                        | 997                         | 35.4431        | 17.7489                    | 0.1672    | 0.2864    | \(R[\tau_i{(C9–H14)+(C10–H15)}]+\tau_0{(C31–H59)}\) |
| 95                | 1039                        | 1002                        | 8.4278         | 4.2873                     | 0.1672    | 0.2866    | \(R[\tau_i{(C9–H14)+(C10–H15)}]+\tau_0{(C31–H59)}\) |
| 96                | 1046                        | 1009                        | 126.0290       | 1.9915                     | 0.6073    | 0.7557    | \(\tau_0{(C35–H39)}+\tau_0{(C44–H64)}\) |
| 97                | 1059                        | 1022                        | 33.1226        | 2.1114                     | 0.4155    | 0.5871    | \(\rho{(H5–C1–H54)+(H6–C4–H53)}\) |
| Mode of Vibration | Calculated freq. (cm\(^{-1}\)) | Scaled freq. (cm\(^{-1}\)) | Intensity (IR) | Raman Activity (A\(^2\)/AMU) | P-Depolar | U-Depolar | Vibration Descriptions |
|-------------------|---------------------------------|-----------------------------|--------------|-----------------------------|-----------|-----------|-----------------------|
| 98                | 1063                            | 1025                        | 18.4490      | 3.9559                      | 0.5167    | 0.6813    | \(\rho\{\text{H5–C1–H54}+\text{H6–C4–H53}\}\) |
| 99                | 1073                            | 1036                        | 35.6843      | 5.0462                      | 0.5332    | 0.6956    | \(\rho\{\text{H60–C32–H61}\}+\tau\{\text{C25–H57}\}\) |
| 100               | 1080                            | 1042                        | 89.7051      | 4.9769                      | 0.3299    | 0.4961    | \(\sigma\{\text{H63–C44–H64}\}+\tau\{\text{C31–H59}\}\) |
| 101               | 1095                            | 1056                        | 136.1010     | 0.7854                      | 0.4696    | 0.6391    | \(\rho\{\text{H5–C1–H54}\}+\tau\{\text{C31–H59}\}\) |
| 102               | 1098                            | 1059                        | 166.2400     | 11.3418                     | 0.1308    | 0.2313    | \(\rho\{\text{H23–C22–H55}\}+\tau\{\text{N66–H67}\}\) |
| 103               | 1099                            | 1060                        | 20.1595      | 4.0721                      | 0.6895    | 0.8023    | \(\sigma\{\text{H60–C32–H61}\}\) |
| 104               | 1110                            | 1071                        | 112.4260     | 3.4367                      | 0.6435    | 0.7831    | \(\tau\{\text{C25–H57}\}+\tau\{\text{C48–H51}\}\) |
| 105               | 1134                            | 1094                        | 50.6433      | 1.4808                      | 0.6699    | 0.8023    | \(\rho\{\text{H23–C22–H55}\}\) |
| 106               | 1137                            | 1097                        | 3.1928       | 11.8999                     | 0.4336    | 0.6049    | \(\tau\{\text{C25–H57}\}+\tau\{\text{C48–H51}\}\) |
| 107               | 1149                            | 1108                        | 56.3226      | 2.2632                      | 0.7221    | 0.8386    | \(\tau\{\text{C38–H41}\}+\tau\{\text{C35–H39}\}\) |
| 108               | 1155                            | 1115                        | 49.6164      | 5.1102                      | 0.1736    | 0.2958    | \(\tau\{\text{C38–H41}\}+\tau\{\text{C35–H39}\}\) |
| 109               | 1166                            | 1124                        | 157.1440     | 2.4269                      | 0.3111    | 0.4745    | \(\tau\{\text{H23–C22–H55}\}\) |
| 110               | 1173                            | 1131                        | 16.6593      | 8.2204                      | 0.3965    | 0.5679    | \(\tau\{\text{H23–C22–H55}\}\) |
| 111               | 1175                            | 1133                        | 2.3943       | 6.4109                      | 0.2135    | 0.3519    | \(\tau\{\text{H23–C22–H55}\}\) |
| 112               | 1184                            | 1142                        | 34.6672      | 3.0060                      | 0.1732    | 0.2952    | \(\tau\{\text{H23–C22–H55}\}\) |
| 113               | 1188                            | 1147                        | 43.9884      | 7.7630                      | 0.333     | 0.4997    | \(\tau\{\text{H23–C22–H55}\}\) |
| 114               | 1206                            | 1164                        | 11.9658      | 6.8856                      | 0.2334    | 0.3785    | \(\tau\{\text{H6–C4–H53}\}\) |
| 115               | 1211                            | 1168                        | 25.3097      | 4.1027                      | 0.7452    | 0.8540    | \(\tau\{\text{C35–H39}\}+\tau\{\text{O47–H52}\}\) |
| 116               | 1215                            | 1172                        | 25.1188      | 1.4384                      | 0.5065    | 0.6724    | \(\tau\{\text{C29–H56}\}+\tau\{\text{H69–C57}\}\) |
| 117               | 1226                            | 1182                        | 75.4750      | 4.3360                      | 0.3778    | 0.5484    | \(\sigma\{\text{H6–C4–H53}\}\) |
| 118               | 1231                            | 1188                        | 3.4134       | 5.1049                      | 0.49      | 0.6577    | \(\sigma\{\text{H6–C4–H53}\}\) |
| 119               | 1238                            | 1194                        | 21.4173      | 3.4418                      | 0.4371    | 0.6083    | \(\tau\{\text{C21–H69}\}+\tau\{\text{C22–H57}\}\) |
| 120               | 1249                            | 1205                        | 7.4251       | 3.5831                      | 0.7498    | 0.8570    | \(\tau\{\text{N17–H18}\}\) |
| Mode of Vibrations | Calculated freq. (cm$^{-1}$) | Scaled freq. (cm$^{-1}$) | Intensity (IR) | Raman Activity (A$^3$/AMU) | P-Depolar | U-Depolar | Vibration Descriptions |
|-------------------|-----------------------------|--------------------------|---------------|---------------------------|-----------|-----------|-----------------------|
| 121               | 1255                        | 1211                     | 4.0754        | 10.9347                   | 0.4474    | 0.6182    | R[ν$_r$((C8–H13)+(C11–H16))]+τ$_0$(C29–H56) |
| 122               | 1257                        | 1212                     | 70.5904       | 1.9949                    | 0.5824    | 0.7361    | τ$_r$(C19–H65)+τ$_0$(C29–H56) |
| 123               | 1267                        | 1223                     | 1.5661        | 1.9962                    | 0.5696    | 0.7258    | R[ν$_r$((C8–H13)+(C11–H16))]+τ$_0$(C38–H41) |
| 124               | 1270                        | 1225                     | 18.3993       | 3.9010                    | 0.1162    | 0.2081    | R[ν$_r$((C8–H13)+(C11–H16))]+τ$_r$(N17–H18) |
| 125               | 1277                        | 1232                     | 10.8100       | 6.1822                    | 0.5225    | 0.6863    | τ$_r$(C22–H55)+τ$_0$(C26–H58) |
| 126               | 1285                        | 1240                     | 15.6778       | 34.5606                   | 0.2229    | 0.3645    | σ(H5–C1–H54)+τ$_r$(C19–H65) |
| 127               | 1295                        | 1249                     | 3.3826        | 8.1360                    | 0.6737    | 0.8050    | τ$_r$(C34–H40)+τ$_0$(C36–H42) |
| 128               | 1309                        | 1263                     | 2.2803        | 3.4565                    | 0.7478    | 0.8557    | τ$_r$(O48–H51)+τ$_0$(C49–H50) |
| 129               | 1312                        | 1266                     | 13.5413       | 8.0947                    | 0.4425    | 0.6135    | τ$_r$(C25–H57)+τ$_0$(C19–H65) |
| 130               | 1320                        | 1274                     | 17.1810       | 6.9844                    | 0.4908    | 0.6584    | τ$_r$(C26–H58)+τ$_0$(C25–H57)+σ(H5–C1–H54) |
| 131               | 1327                        | 1280                     | 17.2994       | 88.2025                   | 0.2209    | 0.3619    | R[τ$_r$(C11–H16)]+σ(C4–H6–C53) |
| 132               | 1335                        | 1288                     | 2.3981        | 0.8176                    | 0.3727    | 0.5430    | τ$_r$(C29–H56)+τ$_0$(C24–H27) |
| 133               | 1345                        | 1297                     | 28.9747       | 0.5832                    | 0.5589    | 0.7171    | σ(H5–C1–H54)+τ$_r$(C21–H59) |
| 134               | 1349                        | 1302                     | 4.8518        | 0.2134                    | 0.6944    | 0.8196    | τ$_r$(C35–H39)+τ$_0$(C37–H62) |
| 135               | 1357                        | 1309                     | 9.8717        | 21.1475                   | 0.4322    | 0.6036    | τ$_r$(C29–H56)+τ$_0$(C31–H59) |
| 136               | 1362                        | 1314                     | 7.8592        | 7.1674                    | 0.5988    | 0.7491    | τ$_r$(C35–H39)+τ$_0$(C44–H63) |
| 137               | 1363                        | 1315                     | 42.9365       | 12.4310                   | 0.6319    | 0.7744    | τ$_r$(C1–H54)+τ$_0$(C19–H65) |
| 138               | 1366                        | 1318                     | 18.9050       | 16.9853                   | 0.3581    | 0.5274    | τ$_r$(C29–H56)+τ$_0$(C26–H58) |
| 139               | 1369                        | 1321                     | 7.1778        | 4.2650                    | 0.0134    | 0.0264    | τ$_r$(C37–H62)+τ$_0$(C29–H56) |
| 140               | 1376                        | 1328                     | 12.4767       | 2.5680                    | 0.7129    | 0.8324    | τ$_r$(C29–H56)+τ$_0$(C25–H57) |
| 141               | 1378                        | 1330                     | 12.3156       | 10.8487                   | 0.618    | 0.7639    | τ$_r$(C19–H65)+τ$_0$(C25–H57) |
| 142               | 1388                        | 1340                     | 19.7655       | 13.4833                   | 0.4421    | 0.6131    | σ(H5–C1–H54)+τ($r$(C21–H69)+τ$_0$(C24–H27) |
| Mode of Vibrations | Calculated freq. (cm\(^{-1}\)) | Scaled freq. (cm\(^{-1}\)) | Intensity (IR) | Raman Activity (Å\(^2\)/AMU) | P-Depolar | U-Depolar | Vibration Descriptions |
|-------------------|-------------------------------|--------------------------|----------------|-------------------------------|-----------|-----------|------------------------|
| 143               | 1395                          | 1346                     | 4.0199         | 4.6797                        | 0.5911    | 0.7430    | \(\tau_i(O_{45}–H_{46})^+\) + \(\tau_0(C_{36}–H_{42})\) |
| 144               | 1396                          | 1347                     | 9.0859         | 7.2537                        | 0.6481    | 0.7865    | \(\tau_i(O_{45}–H_{46})^+\) + \(\tau_i(C_{21}–H_{69})\) + \(\sigma(H_{63}–C_{44}–H_{64})\) |
| 145               | 1406                          | 1356                     | 7.8833         | 8.0503                        | 0.3728    | 0.5431    | \(\tau_i(O_{45}–H_{46})^+\) + \(\tau_i(C_{44}–H_{63})\) + \(\tau_0(C_{36}–H_{42})\) |
| 146               | 1409                          | 1359                     | 4.4669         | 3.6265                        | 0.3185    | 0.4831    | \(\tau_i(C_{25}–H_{57})^+\) + \(\tau_i(C_{36}–H_{42})\) + \(\tau_i(C_{21}–H_{69})\) |
| 147               | 1413                          | 1363                     | 15.9054        | 11.0065                       | 0.2466    | 0.3956    | \(\tau_i(C_{37}–H_{62})^+\) + \(\tau_0(C_{21}–H_{69})\) |
| 148               | 1415                          | 1365                     | 39.1527        | 5.8163                        | 0.3634    | 0.5340    | \(\sigma(H_{63}–C_{44}–H_{64})^+\) + \(\tau_0(C_{36}–H_{42})\) |
| 149               | 1416                          | 1366                     | 19.4783        | 14.6588                       | 0.2459    | 0.3948    | \(\tau_i(C_{34}–H_{40})^+\) + \(\tau_0(C_{37}–H_{62})\) |
| 150               | 1422                          | 1372                     | 47.4160        | 5.8163                        | 0.6639    | 0.7980    | \(\tau_0(C_{26}–H_{58})\) + \(\sigma(H_{63}–C_{44}–H_{64})^+\) + \(\tau_0(C_{36}–H_{42})\) |
| 151               | 1424                          | 1374                     | 17.2198        | 4.0180                        | 0.2907    | 0.4505    | \(\sigma(H_{39}–C_{35}–H_{52})^+\) + \(\tau_0(C_{21}–H_{69})\) |
| 152               | 1429                          | 1379                     | 23.3366        | 1.7898                        | 0.4553    | 0.6258    | \(\tau_i(C_{34}–H_{40})^+\) + \(\tau_0(C_{37}–H_{62})\) |
| 153               | 1431                          | 1381                     | 5.6117         | 1.9203                        | 0.7293    | 0.8434    | \(\sigma(H_{63}–C_{44}–H_{64})^+\) + \(\tau_0(C_{36}–H_{42})\) |
| 154               | 1447                          | 1396                     | 51.1543        | 4.1365                        | 0.5039    | 0.6701    | \(\tau_0(C_{38}–H_{41})^+\) + \(\tau_0(C_{49}–H_{50})\) |
| 155               | 1459                          | 1407                     | 3.0744         | 18.2969                       | 0.3165    | 0.4808    | \(\sigma(H_{60}–C_{32}–H_{61})\) |
| 156               | 1485                          | 1432                     | 9.0244         | 6.7360                        | 0.5698    | 0.7259    | \(\sigma(H_{60}–C_{32}–H_{61})\) |
| 157               | 1486                          | 1434                     | 17.7741        | 22.8194                       | 0.6586    | 0.7942    | \(\sigma(H_{5}–C_{1}–H_{54})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 158               | 1498                          | 1445                     | 31.6135        | 83.9059                       | 0.4483    | 0.6191    | \(\sigma(H_{5}–C_{1}–H_{54})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 159               | 1499                          | 1446                     | 1.9825         | 8.4943                        | 0.739     | 0.8499    | \(\sigma(H_{23}–C_{22}–H_{55})^+\) + \(\tau_i(C_{10}–H_{15})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 160               | 1505                          | 1452                     | 2.3109         | 7.5102                        | 0.7445    | 0.8536    | \(\sigma(H_{63}–C_{44}–H_{64})^+\) + \(\tau_i(C_{10}–H_{15})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 161               | 1507                          | 1454                     | 2.0456         | 50.9273                       | 0.6155    | 0.7620    | \(\sigma(H_{23}–C_{22}–H_{55})^+\) + \(\tau_i(C_{10}–H_{15})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 162               | 1531                          | 1477                     | 8.9991         | 4.3501                        | 0.75      | 0.8571    | \(\sigma(C_{7}–N_{17}–H_{18})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 163               | 1611                          | 1554                     | 2.2164         | 119.3097                      | 0.3907    | 0.5618    | \(\sigma(C_{7}–N_{17}–H_{18})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 164               | 1637                          | 1579                     | 2.6194         | 283.5082                      | 0.2289    | 0.3725    | \(\sigma(C_{7}–N_{17}–H_{18})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 165               | 1652                          | 1594                     | 38.9286        | 4.9743                        | 0.7313    | 0.8448    | \(\sigma(C_{7}–N_{17}–H_{18})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| 166               | 1670                          | 1612                     | 8.0093         | 22.4639                       | 0.3473    | 0.5155    | \(\sigma(C_{7}–N_{17}–H_{18})^+\) + \(\tau_0(N_{17}–H_{18})\) |
| Mode of Vibrations | Calculated freq. (cm⁻¹) | Scaled freq. (cm⁻¹) | Intensity (IR) | Raman Activity (A²/AMU) | P- Depolar | U- Depolar | Vibration Descriptions |
|-------------------|-------------------------|--------------------|--------------|------------------------|------------|------------|-----------------------|
| 167               | 1698                    | 1638               | 10.2616      | 47.9569                | 0.0694     | 0.1298     | σ(H60–C32–H61)        |
| 168               | 1735                    | 1674               | 124.9900     | 77.8820                | 0.0838     | 0.1546     | ρ(C24–H27–C28)        |
| 169               | 2962                    | 2858               | 73.8483      | 46.1947                | 0.3802     | 0.5510     | τi(C1–H54)            |
| 170               | 2968                    | 2864               | 30.7878      | 257.1128               | 1697       | 0.2902     | τ0(C19–H65)           |
| 171               | 2980                    | 2875               | 12.9742      | 39.7241                | 0.2464     | 0.3954     | τ0(C36–H42)           |
| 172               | 3002                    | 2896               | 13.1860      | 29.3710                | 0.2112     | 0.3487     | τ0(C37–H62)           |
| 173               | 3003                    | 2897               | 63.2418      | 138.8816               | 0.2238     | 0.3658     | τ0(C21–H69)           |
| 174               | 3004                    | 2899               | 21.3855      | 91.4456                | 0.1863     | 0.3141     | τ0(C29–H56)           |
| 175               | 3011                    | 2905               | 33.8790      | 92.2179                | 0.2633     | 0.4169     | τ0(C35–H39)           |
| 176               | 3012                    | 2906               | 53.4165      | 175.3515               | 0.1299     | 0.2300     | τ0(C34–H40)           |
| 177               | 3047                    | 2940               | 34.5134      | 86.1906                | 0.1785     | 0.3029     |                      |
| 178               | 3050                    | 2943               | 30.4769      | 112.3494               | 0.6007     | 0.7506     | νas(H6–C4–H53)        |
| 179               | 3053                    | 2946               | 30.9161      | 89.1537                | 0.0899     | 0.1649     | σ(H23–C22–H55)        |
| 180               | 3061                    | 2954               | 3.1561       | 114.7644               | 0.1041     | 0.1885     | τ0(C26–H58)           |
| 181               | 3074                    | 2966               | 23.9359      | 92.5846                | 0.0623     | 0.1173     | ν0(H63–C44–H64)       |
| 182               | 3092                    | 2983               | 28.8788      | 68.2005                | 0.3142     | 0.4782     | ν0(H63–C44–H64)       |
| 183               | 3093                    | 2985               | 32.7954      | 45.9705                | 0.4688     | 0.6384     | ν0(H23–C22–H55)       |
| 184               | 3097                    | 2988               | 16.1497      | 106.4138               | 0.1893     | 0.3183     | τ0(C38–H41)           |
| 185               | 3107                    | 2997               | 30.0290      | 137.7424               | 0.3044     | 0.4667     | τ0(C1–H5)             |
| 186               | 3130                    | 3020               | 12.7610      | 50.8469                | 0.6892     | 0.8160     | νas(H63–C44–H64)       |
| 187               | 3141                    | 3031               | 9.4776       | 32.4709                | 0.4884     | 0.6562     | τ0(C31–H59)           |
| 188               | 3164                    | 3053               | 13.9988      | 182.9783               | 0.1487     | 0.2590     | τ0(C31–H59)+          |
| 189               | 3174                    | 3062               | 1.2693       | 33.8895                | 0.7491     | 0.8566     | R[τ0(C8–H13)+         |
|                   |                         |                    |              |                        |           |            | (C11–H16)]            |
| 190               | 3181                    | 3069               | 3.4570       | 128.7092               | 0.7021     | 0.8250     | R[τ0(C9–H14)+         |
|                   |                         |                    |              |                        |           |            | (C11–H16)]            |
| 191               | 3191                    | 3079               | 33.4769      | 75.4914                | 0.7287     | 0.8430     | R[τ0(C8–H13)+         |
|                   |                         |                    |              |                        |           |            | (C10–H15)]            |
| 192               | 3202                    | 3090               | 29.9950      | 357.6723               | 0.1419     | 0.2485     | R[τ0(C9–H14)+         |
|                   |                         |                    |              |                        |           |            | (C11–H16)]            |
| 193               | 3207                    | 3094               | 10.4631      | 106.5830               | 0.2910     | 0.4508     | τ0(C24–H27)           |
| 194               | 3257                    | 3142               | 3.2147       | 56.4511                | 0.7223     | 0.8388     | νas(H60–C32–H61)      |
| 195               | 3498                    | 3375               | 1.7372       | 164.5797               | 0.1475     | 0.2570     | τ0(N17–H18)           |
| 196               | 3560                    | 3434               | 255.1180     | 219.8025               | 0.2155     | 0.3546     | νas(H67–N66–H68)      |
| 197               | 3591                    | 3465               | 0.7554       | 71.6149                | 0.5863     | 0.7392     | τ0(C47–H52)           |
| 198               | 3727                    | 3596               | 64.5414      | 72.1314                | 0.0551     | 0.1045     |                      |
| 199               | 3741                    | 3610               | 55.4321      | 12.5077                | 0.2566     | 0.4084     | τ0(O49–H50)           |
| 200               | 3785                    | 3652               | 92.7042      | 34.7794                | 0.3617     | 0.7743     | τ0(O45–H46)           |
| 201               | 3785                    | 3652               | 44.0067      | 112.6047               | 0.0976     | 0.1778     | τ0(O45–H46)+          |
Similar types of results were obtained by using higher basis set combination with the same functional.

4. Discussions
The vibrations in the domain of 3093-2997 cm\(^{-1}\) occurring at the active modes of vibrations 193-185 as obvious from the Table 1, are ascertained to be C-H stretching which in covenant with earlier reported characteristic domain of 3100–3000 cm\(^{-1}\) [18] seemed due to the availability of aromatic ring. The vibrational modes 134-95 shows the frequency domain of 1301-1002 cm\(^{-1}\) which correspond to C–H in plane bending frequencies appearing in line with the reported domain of 1300–1000 cm\(^{-1}\) [19]. The C–H out of plane bending vibrations have been reflected in the domain of 1000–750 cm\(^{-1}\) [20] which are well matched with the theoretical vibrations occurred at the active modes 94-68 in the domain of 997-750 cm\(^{-1}\). Thus, the theoretically evaluated regions for C–H vibrations are well corresponding with their experimental consequence. The C–C stretching vibrations in the selected compound are set up in the domain of 1593-1396 cm\(^{-1}\) corresponding to the vibrational mode 165-154. The low region frequencies of other vibrational modes which are hardly observed in experiments have also been calculated through the said theoretical approach. The strongest Raman activity has been observed at 3202 cm\(^{-1}\) which is the characteristics of this molecule.

5. Conclusions
The optimized geometry obtained by molecular modeling applying density functional theory at B3LYP/6-31+G(d,p) level exhibits the vibrational spectroscopic characteristics which are in good agreement with other reported results which reveals that the applied theoretical model and its higher basis set combination is a compatible quantum chemical analysis for the theoretical evaluation of vibrational spectroscopy of the said natural product. The strongest IR active & Raman activity has been observed to be occurred at the wave numbers 388 & 3202 cm\(^{-1}\) respectively which may be applicable as characteristic factor for the said molecule.

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