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Experimental, anticancer activity and density functional theory study on the vibrational spectra of 2-(4-fluorobenzylideneamino) propanoic acid

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ABSTRACT

2-(4-Fluorobenzylideneamino) propanoic acid was synthesized through the reaction of 4-fluorobenzaldehyde and α -alanine in refluxing EtOH. Its structure was verified by ¹H NMR, FTIR and Raman spectroscopy. The ground-state geometries were optimized at B3LYP/6-31G*, B3LYP/6-31+G** and B3LYP/6-31G** level without symmetry constrains. The vibrational wavenumbers of 4-FA were calculated at same level. The scaled theoretical spectra using B3LYP methods are in a good agreement with the experimental ones. The title compound was tested for anticancer activity of the Hela cell line (using an MTT viability assay) with an IC₅₀ 166.6 µg/mL.

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1. Introduction

Malignant tumor, i.e., cancer is a dreadful menace to human beings [1]. So the development of potential and effective anticancer drugs has become one of the most intensely persuaded goals of contemporary medicinal chemistry. The role of schiff bases as intermediate products in biologically important reactions is well known and documented [2]. Derivatives of amino acids and pyridoxal or salicylaldehyde have been widely studied [3,4]. In addition, fluoroaromatic compounds have become increasingly important in view of their application as agrochemicals, drugs, textile chemicals, etc. [5] and the carbon-fluorine bonds enhances certain molecular properties (e.g., lipid solubility, bioactivity, reduced toxicity and oxidative stability). As this kind of fluoroaromatic. Pfluorobenzaldehyde is very important due to its extensive use as intermediate for pharmaceutical [6]. This gave a great impetus to the search for potential pharmacologically active 4-fluorobenzidine α -alanine Schiff base (4-FA) derived from 4-fluorobenzaldehyde and α -alanine. On the basis of its ¹H NMR spectra and element analyses the Schiff base structure immediately could be confirmed

(Fig. 1) [7]. In addition, we wish to report a theoretical study of the vibrational properties of 4-FA. Many study results have indicated that density-functional theory (DFT) is a powerful method for predicting the geometry and harmonic vibration of organic compounds [8–13]. DFT is a useful method for the investigation of large molecules [11].

In our present work, the ground-state geometries of 4-FA were optimized at B3LYP/6-31G**, B3LYP/6-31G* and B3LYP/6-31+G** levels, respectively. Analytical vibrational frequencies were calculated at the same level.

The MTT assay was used for the quantification of living, metabolically active cells in initial experiments. Cellular dehydrogenases metabolize MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) to a purple formazan dye, which is then solubilized in DMSO and measured photometrically at 570 nm. After incubation of cells with fresh medium with 0.25 mg/mL MTT for 1 h, the medium was aspirated, cells were washed once with PBS (+/+), and the formazan crystals were solubilized in DMSO. Viability was calculated as percentage of formazan formation in cells interacted with 4-FA compared to mock-treated cells.

2. Experiment

All materials and solvents were obtained from commercial suppliers and used without further purification. 4-Fluorobenzaldehyde

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Fig. 1. The geometry and atom numbering of 4-FA.

was from Sigma. ¹H NMR spectra were recorded on a AS 300 (VAR-IAN) using TMS as an internal standard. Compound dissolved in DMSO- d_6 . Element analyses were obtained on a PE 2400 CHN analyzer. Melting point was measured in WRS-1B digital melting point instrument. Infrared spectra of the compound dispersed in KBr pellet in the range of 4000–400 cm⁻¹ were recorded on an IR-Spectra One (PE). The Raman spectra of powder sample were acquired on with Renishaw RM1000 spectrometer using Nd:YAG laser as excitation source (785 nm) with an output of about 200 mW. The spectral regions were 400–3500 cm⁻¹.

Synthesis of 4-FA: In a 1:1 molar ratio, α -alanine (0.7127 g, 8×10^{-3} mol) and potassium hydroxide (0.4489 g, 8×10^{-3} mol) were added in 30 mL absolute EtOH The solution of α -alanine potassium salt was filtered after the mixture was refluxed under stirring for 1 h and left to stand at room temperature [14]. Under stirring and nitrogen atmosphere, 4-fluorobenzaldehyde (1.00 mL, 10×10^{-3} mol) in 10 mL anhydrous EtOH was added. After 3 h, the solvent was removed under reduced pressure and the remaining solid residue was dissolved in EtOH (30 mL). Then we used concentrated H₂SO₄ to transform COOK to COOH [15]. After acidification of the resulting solution, the precipitated crude product was filtered, washed with petroleum ether, dried and recrystallized [16]. Yield: 91.5%. mp: 149–151 °C. Anal. Calc. for C₁₀H₁₀FNO₂ (shown in Fig. 1): C, 61.52; H, 5.16; N, 7.17. Found: C, 61.40; H, 5.12; N, 7.05. ¹H NMR: δ 8.22(1H, bs, CH=N), 7.74(2H, dd, H-2), 7.23(2H, t, H-3), 3.69(1H, m, CH-CH₃), 1.25 (3H, d, CH-CH₃).

Biological testing: Cells were allowed to grow to 60-80% confluence under conditions of 5% CO_2 at 37 °C. A stock solution of each compound was prepared in 1 mL of DMSO followed by dilution with fresh medium. A 96-well plate was set up for compound with six in-plate replicates of the three concentrations on the plate. Cell solution (200 $\mu L, 5 \times 10^4$ cells/mL, 1×10^4 cells/well) was plated and initially incubated for 24 h, after which the media were removed and 100 µL of media containing 1% DMSO was added. Plates were incubated at 5% CO₂ at 37 °C for 3 days, after which the cells were washed with 200 µL PBS, 200 µL of 0.5 mg/mL MTT solution was added to each well, and the cells were incubated for 2 h at 37 °C at 5% CO₂. The MTT solution was then removed, the wells were washed again with PBS, 200 µL DMSO solution was added and the plates were incubated in the dark for 10 min. Absorbance readings were taken at 570 nm using an Anthos III microplate spectrophotometer. The data were processed with the aid of Microsoft Excel 2000 and the % growth at each compound concentration was calculated as follows: % grown = $\frac{\text{compound}-\text{blank}}{\text{control}-\text{blank}}$ compound is the mean absorbance of the inhibitor and the cell culture, blank is the absorbance of the media alone and control is the absorbance of the media with cells. IC₅₀ was defined as the compound concentration, which caused 50% inhibition of the growth of the treated cells compared to the control cells. The inhibition rates are 17.2, 19.5 and 24.0 for the 4-FA with the concentrations of 266.7, 133.4 and 66.7 μ g/mL, respectively, and the IC₅₀ is 166.6 μ g/mL against Hela cell.

3. Calculation

The DFT calculations were employed with the Becke-Lee-Yang–Parr's three-parameter hybrid functional (B3LYP) [17] method in this study. The same basic sets (6-31G** and 6-31G*) [18] were employed in the B3LYP calculations and the geometry optimizations were performed without symmetry constrain. It is known that ab initio and DFT potentials systematically overestimate the vibrational wavenumbers [19]. These discrepancies can be corrected either by computing an harmonic corrections explicitly or by introducing a scaled field [20] or directly scaling the calculated wavenumbers with proper factor [21]. Therefore, we have used the scaling factor values of 0.9614, 0.9700 and 0.9670 for B3LYP/6-31G*, B3LYP/6-31 + G** and B3LYP/6-31G** methods, respectively [21]. All calculations were performed with the Gaussian 03W program suit [22]. The assignment of the calculated wavenumbers is aided by the animation option of Gauss View 3.0 graphical interface for Gaussian programs, which gives a visual presentation of the shape of the vibrational modes [23,24].

4. Results and discussion

The schematic depiction of 4-FA and optimized structure are shown in Fig. 1, and the optimized bond lengths, bond angles and dihedral angles of 4-FA are shown in Table 1.

The carboxylic group is practically planar with the asymmetrical C(12)=O(13) 1.212 and C(12)-O(14) 1.353 Å distances, which are consistent with the double and single C–O bonds, respectively [25]. From Table 1, the bond lengths, bond angles and dihedral angles calculated at B3LYP/6-31+G^{**} level are in agreement with those calculated at B3LYP/6-31G^{*} and B3LYP/6-31G^{**} levels.

The values of zero-point vibrational energy, sum of electronic and zero-point energy, $E_{\rm HOMO}$, $E_{\rm LUMO}$, thermal correction to energy for 4-FA are listed in Table 2. The HOMO energy calculated by B3LYP/6-31+G** are 0.4 eV higher than by B3LYP/6-31G* and B3LYP/6-31G**. The dipole moment calculated using B3LYP/6-31+G** level is 0.3 D higher than those using B3LYP/6-31G* and B3LYP/6-31G** levels.

Figs. 2 and 3 show the observed FTIR and Raman spectra, respectively. One can notice that many bands have shoulders or are quite broad because of the overlapping of two or more unresolved components. We have listed the strongest peaks and noted the presence of appropriate shoulders.

The FTIR and Raman spectra of 4-FA were fully interpreted on the basis of the IR and Raman spectra calculated at B3LYP/6- $31+G^{**}$, B3LYP/6- $31G^{**}$ and B3LYP/6- $31G^{*}$ levels, respectively. The calculated wavenumbers scaled by factor of 0.9700 at B3LYP/6- $31+G^{**}$, 0.9670 at B3LYP/6- $31G^{**}$ and 0.9614 at B3LYP/6- $31G^{*}$ levels, intensity and assignments are listed in Table 3, respectively. The agreement between the experimental and scaled theoretical frequencies is quite good in general.

Table 1

Selected bond lengths, bond angles, dihedral angles of compound 4-FA.

Parameters	B3LYP/6-31 + G**	B3LYP/6-31G*	B3LYP/6-31G*		
Bond length (Å)					
C(6)-F(7)	1.358	1.348	1.348		
C(1)-C(2)	1.396	1.394	1.394		
C(2)-C(3)	1.403	1.403	1.402		
C(3)-C(4)	1.407	1.406	1.406		
C(4)-C(5)	1.391	1.390	1.389		
C(5)-C(6)	1.393	1.394	1.394		
C(6)-C(1)	1.389	1.390	1.390		
C(3)-C(8)	1.474	1.472	1.472		
C(8)-N(9)	1.275	1.274	1.275		
N(9)-C(10)	1.460	1.459	1.459		
C(10)-C(12)	1.531	1.532	1.532		
C(10)-C(11)	1.541	1.540	1.540		
C(12)-C(13)	1.212	1.210	1.210		
C(12)-O(14)	1.353	1.354	1.353		
C(10)-H(20)	1.095	1.096	1.095		
O(14)-H(24)	0.972	0.976	0.972		
C(11)-H(21)	1.094	1.095	1.094		
Bond angle (°)					
C(1)-C(2)-C(3)	121.1	121.0	121.0		
C(2)-C(3)-C(8)	119.3	119.6	119.6		
C(4)-C(3)-C(8)	121.6	121.4	121.4		
C(3)-C(8)-H(19)	114.8	114.7	114.8		
C(3)-C(8)-N(9)	122.4	122.2	122.1		
C(8)-N(9)-C(10)	121.1	120.9	120.9		
N(9)-C(10)-C(11)	118.8	118.7	118.9		
N(9)-C(10)-C(12)	108.6	108.7	108.6		
N(9)-C(10)-H(20)	106.3	106.5	106.6		
C(11)-C(10)-H(20)	108.7	108.6	108.7		
C(12)-C(10)-H(20)	104.1	104.3	104.2		
C(10)-C(12)-O(13)	124.8	125.0	125.0		
C(14)-C(12)-O(13)	122.8	122.9	123.0		
C(12)-O(14)-H(24)	107.1	106.0	106.0		
Dihedral angle (°)					
C(4)-C(3)-C(8)-N(9)	-0.6	-0.8	-0.8		
C(3)-C(8)-N(9)-C(10)	-179.6	180.0	180.0		
C(8)-N(9)-C(10)-C(12)	-126.3	-122.9	-123.1		
C(8)-N(9)-C(10)-C(11)	-0.6	2.3	2.1		
C(8)-N(9)-C(10)-H(20)	122.2	125.2	125.2		
N(9)-C(10)-C(12)-O(13)	-128.4	-130.0	-129.3		
C(10)-C(12)-O(14)-H(24)	178.8	178.4	178.5		





1500

1000

500



Figs. 4 and 5 show the unscaled calculated IR and Raman spectra of 4-FA at B3LYP/6-31+G** (a), B3LYP/6-31G** (b) and B3LYP/6-31G* (c) levels, respectively.

The calculations show that the strong band at 3643 cm⁻¹ in FTIR is associated with the stretching vibration of O–H of carboxyl, which is observed at 3498 cm^{-1} . The bands near 3100 cm^{-1} can be attributed to the aromatic C–H stretching [26]. The band of C–H stretching vibrational mode for benzene appears at 3080 cm⁻¹ in FTIR and 3083 cm⁻¹ in Raman spectra. The very weak intense peak at 2974 cm⁻¹ in FTIR and weak intense peak at 2976 cm⁻¹ in Raman spectra are attributed to the C10-H20 stretching vibration. The C–H aromatic stretches is very weak, which is observed at 3040 cm⁻¹ in FTIR and 3044 cm⁻¹ in Raman spectra, respectively [27]. The band observed at 2936 cm⁻¹ in FTIR and 2939 cm⁻¹ in Raman spectra are assigned to the symmetric stretching vibration of CH₃ mixed with the stretching vibration of C8–H19. The medium intense band at 1455 cm⁻¹ in FTIR and 1456 cm⁻¹ in Raman spectra are assigned to the asymmetric deformation of CH₃. The medium band at 1379 cm^{-1} , the strong peak at 1362 cm^{-1} in FTIR and the medium band at 1383 cm^{-1} , the very weak band at 1365 cm^{-1} in Raman spectra are assigned to the symmetric deformation of CH₃ mixed with in-plane wagging of C8-H19.

Та	bl	e 2	

Thermodynamic parameter for 4-FA.

	D2IVD/C 21 + C**	POLVD/C 21C*	D2IVD/C 21C**
	DSLIP/0-51+G	DSLIP/0-SIG	DSLIP/0-SIG
Thermodynamic parameter ^a			
Zero-point vibrational energy (kJ mol ⁻¹)	486.0	488.5	487.6
Thermal correction to energy (kJ mol ⁻¹)	519.9	522.2	521.4
Entropy (J mol ^{-1} K ^{-1})	486.8	485.5	485.7
$C_V (J mol^{-1} K^{-1})$	200.8	199.6	200.1
E _{HOMO} (eV.)	-6.905	-6.514	-6.519
E _{LUMO} (eV)	-1.767	-1.325	-1.335
Dipole moment (D)	3.026	2.691	2.717
Sum of electronic and zero-point energy (kJ mol ⁻¹)	-692.0	-691.9	-692.0

0

3500

3000

2500

^a Unscaled for 298 K and 1 atm.

Table 3 The observed fundamentals and calculated wavenumbers (cm⁻¹), FTIR and Raman intensity and assignments for 4-FA.

Descriptions	Calculated					Observed				
	B3LYP/6-31 + G**	B3LYP/6-31 + G**a	B3LYP/6-31G*	B3LYP/6-31G*a	B3LYP/6-31G**	B3LYP/6-31G**a	IR intensity ^b	Raman intensity	IR exp	Raman exp
vs(O-H)	3756	3643	3685	3543	3753	3629	52.8	149.8	3498(s)	
v(C–H)benz	3182	3087	3184	3063	3183	3078	10	53.3	3080(vw)	3083(w)
v(C–H)benz	3131	3037	3138	3017	3136	3033	18.8	64	3040(vw)	3044(vw)
v(C10-H20)	3073	2980	3078	2959	3073	2972	9.8	148.9	2974(vw)	2976(w)
$v(CH_3) + v(C8-H19)$	3044	2952	3050	2932	3043	2943	21	27.2	2936(vw)	2939(w)
vs(C=0)	1816	1761	1850	1779	1848	1787	380	5.8	1683(s)	1655(s)
$\nu s(C=N)$	1726	1674	1735	1668	1733	1676	86.2	476.6	1650(s)	1642(vs)
v(C=C)benz	1650	1601	1666	1602	1663	1608	111.3	331.6	1603(vs)	1606(vs)
v(C=C)benz	1635	1586	1642	1579	1640	1586	17.9	30.9	1583(vs)	1596(s)
v(C=C)benz	1544	1498	1561	1501	1556	1505	71.8	35	1508(s)	1511(w)
$\delta as(CH_3)$	1504	1459	1526	1467	1509	1459	7	18.3	1455(m)	1456(m)
v(C=C)benz	1452	1408	1465	1408	1459	1411	6.8	10.8	1404(s)	1420(m)
$\delta s(CH_3) + \rho(C8 - H19)$	1419	1376	1434	1379	1425	1378	19.3	4.3	1379(m)	1383(vw)
$\delta s(CH_3) + \rho(C8-H19)$	1404	1362	1422	1367	1409	1363	4.7	6.7	1362(s)	1365(vw)
v(C=C)benz	1346	1306	1354	1302	1351	1306	2.1	3.5	1309(m)	1313(vw)
ρ (C–H)benz	1321	1281	1329	1278	1320	1276	7.8	23.2	1294(m)	1299(m)
ρ (C–H)benz	1315	1276	1324	1273	1315	1272	16.5	22.9	1276(m)	1279(w)
Def of benz ring(ip) + ν (C–F)	1259	1221	1288	1238	1286	1244	146.9	39.8	1230(vs)	1229(s)
ρ(O-H)	1196	1160	1213	1166	1205	1165	149.5	5	1155(vs)	1158(s)
δ (C–H)benz	1175	1140	1185	1139	1177	1138	35.9	20.8	1129(m)	1133(w)
δ (C–H)benz	1125	1091	1133	1089	1127	1090	16.7	7.8	1095(m)	1100(w)
ν (C9–C10)+ δ (C–H)benz	1113	1080	1122	1079	1116	1079	9	9.8		1081(w)
ν (C10–C11)+ δ (C–H)benz	1097	1064	1105	1062	1101	1065	35.4	5.6	1047(s)	1048(w)
Def of benz ring (ip)	1029	998	1034	997	1033	999	61.9	4.5	1012(m)	1014(vw)
Breath of benz ring	1005	975	1014	975	1012	979	11.2	5.7	975(m)	978(w)
Breath of benz ring	989	959	983	945	985	952	0	0.3	966(w)	969(w)
Breath of benz ring	955	926	947	910	948	917	0.2	1	920(w)	937(vw)
v(N9-C10-C11)	908	881	913	878	911	881	9.9	7.4	888(m)	890(s)
vske of benz ring	882	856	888	851	887	858	16.6	22.8		859(s)
γ (C–H)benz	856	830	853	820	852	824	44.9	1.9	838(vs)	838(w)
γ (C–H)benz	831	806	832	800	831	804	7	5	. ,	822(w)
Def of benz ring (ip)	812	788	817	785	816	789	2.9	4.5	790(m)	795(s)
Def of benz ring (op)	719	697	718	690	718	694	0.3	0.9	712(w)	
Def of benz ring (ip)	650	631	654	629	653	631	7.4	1.2	643(m)	641(w)
ω(O-H)	612	594	624	600	621	601	65.3	4.8		610(w)
Def of benz ring (op)	525	509	532	511	531	513	21	0.6	508(s)	511(vw)
Def of benz ring (op)	516	501	518	497	518	501	20	0.9	483(m)	487(vw)
Def of benz ring (op)	428	415	430	413	431	417	0.6	0.2	. ,	433(vw)
δ(C10-C11-C12)	330	320	328	315	329	318	1.8	2.6		315(vw)
τ(C10-C11)	297	288	302	290	301	291	3.2	1.3		292(vw)
$\delta(C3 - C4 - C8)$	235	228	237	228	236	228	1.5	1.6		232(m)
ω(N9-C10-C11)	226	219	226	218	226	219	1.3	1.7		222(vs)

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Abbreviation: as, asymmetric; s, symmetric; benz, benzene; υ, stretching vibration; def, deformation; τ, torsion; ω, wagging out-of-plane; ρ, wagging in-plane; op, out-of-plane mode; ip, in-plane mode; δ, scissors vibration; δas, asymmetric deformation; δs, symmetric deformation; β, bending in-plane; γ, bending out-of-plane; ske, skeleton; s, strong; w, weak; m, medium; vs, very strong; vw, very weak.

^a Scaling factor: B3LYP/6-31 + G**, 0.97; B3LYP/6-31G**, 0.967; B3LYP/6-31G*, 0.9614.

^b The absolute IR intensity in KM(mol)-1; Raman scattering activity in Å 4 (amu)-1 from B3LYP/6-31G* calculation.



Fig. 4. The unscaled IR spectra of 4-FA at (a) B3LYP/6-31+G**, (b) B3LYP/6-31G* and (c) B3LYP/6-31G** level.

The strong absorption bands of the C=O stretching vibration are observed at 1683 cm⁻¹ in FTIR and 1655 cm⁻¹ in Raman, which are in accordance with the experimental values (1692 and 1640 cm⁻¹) obtained for monoglycine dihydrogenphosphate [28] and dimmer dibenzyl carbamic acid [29], respectively. The discrepancy between simulation and experiment spectra is due to the intermolecular interactions. The strong intense peaks appear at 1650 cm⁻¹ in FTIR and 1642 cm⁻¹ in Raman spectra assigned as the stretching vibration of C=N, which is in accordance with the experimental value (1637 cm⁻¹) obtained for Sal-ala-Mn compound [17]. The intensity of the band observed at 1642 cm⁻¹ in Raman spectra is the strongest one, and the band is also the most intense one of the calculated intensity in Raman spectra.

The bands of C=C stretching vibrations for benzene ring appear at 1603, 1583, 1508, 1404 cm^{-1} in FTIR and 1606, 1596, 1511, 1420 cm⁻¹ in Raman spectra. The bands at 1603, 1583 cm⁻¹ in FTIR



Fig. 5. The unscaled Raman spectra of 4-FA at (a) B3LYP/6-31+G^{**}, (b) B3LYP/6-31G^{*} and (c) B3LYP/6-31G^{**} level.

and 1606 cm^{-1} in Raman spectra are all very strong absorptions. The bands at 1508, 1404 cm^{-1} in FTIR and 1596 cm^{-1} in Raman spectra are strong, and the one at 1420 cm^{-1} in Raman spectra is medium. The strongest band is observed at 1603 cm^{-1} in FTIR, however, the most intense one appears at 1683 cm^{-1} in the calculated IR spectra.

The very strong absorption band at 1230 cm⁻¹ in FTIR and strong band at 1229 cm⁻¹ in Raman are due to the stretching vibration of C–F. The bands are in good agreement with the literature value (1230 cm⁻¹) obtained for 2-fluoro-4, 6-dinitrophenol [30]. The medium bands at 1294, 1276 cm⁻¹ in FTIR and the bands at 1299, 1279 cm⁻¹ in Raman spectra are assigned to the C-H in-plane wagging vibrations for benzene. The bands with medium intensities observed at 1129, 1095 and 1047 cm⁻¹ in FTIR, and the bands with weak intensities appear at 1133, 1100, 1081 and 1048 cm⁻¹ in Raman spectra are assigned to the C–H scissors vibrations for phenyl. The peaks at 975, 966 and 920 cm^{-1} in FTIR and 978, 969 and 937 cm^{-1} in Raman spectra can be assigned to the breathing vibrations of benzene ring. The intensity of the breath vibration of benzene ring is weak, and the band at 975 cm⁻¹ in FTIR is a medium one and the band at 937 cm⁻¹ in Raman spectra is a very weak one. The strong intense peak observed at 859 cm⁻¹ in Raman spectra is attributed to the skeletal vibration of benzene. The medium intensity band obtained at 888 cm⁻¹ in FTIR and strong intensity band obtained at 890 cm⁻¹ in Raman spectra are assigned to the stretching vibration of N9-C10-C11. The very strong intensity band observed at 838 cm⁻¹ in FTIR and weak intensity bands appear at 838 and 822 cm⁻¹ in Raman spectra are assigned to the C–H outplane bending for benzene ring. The bands at 790, 712, 643 cm⁻¹ in FTIR and 795, 641 cm⁻¹ in Raman spectra can be assigned to the inplane deformation of benzene ring. The out-of-plane deformations of benzene ring are observed at 508 and 483 cm^{-1} in FTIR and 511, 487, 433 cm⁻¹ in Raman spectra. The band with very weak intensity at 315 cm⁻¹ in Raman spectra is assigned to the scissors vibration of C10-C11-C12. The band of torsion for C10-C11 is observed at 292 cm⁻¹ in Raman spectra with very weak intensity. The medium peak at 232 cm⁻¹ in Raman spectra is assigned to the out-plane deformation of C3–C4–C8. The peak with very strong intensity at 222 cm⁻¹ in Raman spectra is assigned to the out-of-plane wagging of N9-C10-C11.

5. Conclusion

4-FA obtained in the reaction of 4-fluorobenzaldehyde with αalanine potassium salt in refluxing EtOH. Its structure was verified by ¹H NMR, FTIR and Raman. The mp = 149–151 °C. FTIR and Raman spectra of 4-FA were carried out. The ground-state geometries were optimized without symmetry constrains using the DFT-B3LYP method with 6-31G*, 6-31+G** and 6-31G** basis sets, respectively. The vibrational wavenumbers of 4-FA were calculated on optimized geometry by means of B3LYP/6-31G*, B3LYP/6-31+G** and B3LYP/6-31G**, respectively. After scaled with uniform scaling factors, the predicted spectra are well consistent with experimental spectra. The title compound was assayed for anticancer activity by MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) method. The inhibition rates are 17.2, 19.5 and 24.0 for the 4-FA with the concentrations of 266.7, 133.4 and 66.7 μg/mL, respectively, and the IC₅₀ is 166.6 μg/mL against Hela cell.

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