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Synthesis, Characterization, Crystal Studies of (E)-3-(3-(4-Fluorophenyl)-1-isopropyl-1H-indol-2-yl) Acrylaldehyde

Veerendra Kumar A. Kalalbandi, J. Seetharamappa*
Department of Chemistry, Karnatak University, Dharwad, India
Email: *jseetharam@yahoo.com

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ABSTRACT

We have synthesized and developed single crystals of the title compound (E)-3-(3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl) acrylaldehyde, which is a key intermediate of anti-cholesterol fluvastatin drug. It crystallized under orthorhombic system with a space group $Pna2_1$. The dihedral angle between the indole mean plane and 4-F-phenyl ring was observed to be 111.5 (3)˚ in the title molecule. Further, strong hydrogen bonds were not found in the crystal structure.

Keywords: Single Crystal Structure; X-Ray Diffraction; Intermediate of Fluvastatin; Indoles

1. Introduction

Indole and its derivatives have been a topic of research interest and continue to be one of the dynamic areas of heterocyclic chemistry, particularly due to their natural occurrence and pharmacological activities [1]. A large number of indole derivatives are at the fore as pharmacologically active lead compounds for drug development [2]. Many drugs contain indole moiety, either as a basic prototype or as an attached group to invoke particular properties [3]. The incorporation of indole nucleus, a biologically accepted pharmacophore in medicinal compounds, has made it versatile heterocyclic possessing wide spectrum of biological activities [4,5] like anticancer, antimicrobial, anti-HIV, antitubercular, antiviral, antidepressant, cardiovascular activity, antihypertensive, etc., [6-9]. Furthermore, fluvastatin, which is a synthetic member of the statin class, contains indole moiety in its molecular makeup and the title molecule is its key intermediate.

In the course of synthesizing some fluvastatin derivatives, we have developed single crystals of key intermediate, (E)-3-(3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl) acrylaldehyde and its molecular structure were determined. In the present paper, we report the synthesis, characterization by FTIR, ^{1}H NMR and ^{13}C NMR and its crystal properties.

*Corresponding author.

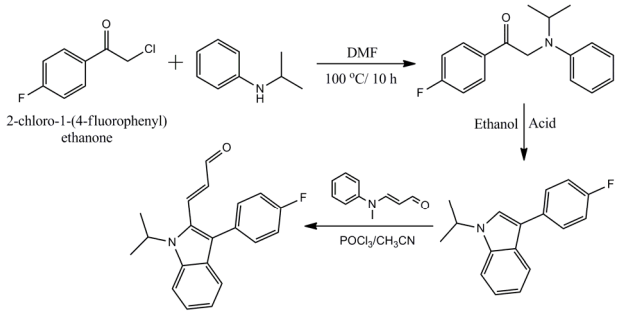
2. Experimental

2.1. Synthesis of the Title Compound

The title compound (E)-3-(3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl) acrylaldehyde was synthesized by following the reported method [10,11]. Friedel-Crafts condensation of fluorobenzene with chloroacetyl chloride in the presence of $AlCl_3$ gave 4-Fluoro phenacyl chloride. Phenacyl chloride was then condensed with N-isopropylaniline in the presence of DMF to yield 1-(4-fluorophenyl)-2-(isopropyl(phenyl)amino) ethanone. Further, this was cyclized by means of $ZnCl_2$ to yield 3-(4- fluorophenyl)-1-isopropyl-1H-indole. The condensation of 3-(4-fluorophenyl)-1-isopropyl-1H-indole with 3-(N-methyl-N-phenylamino) acrolein in the presence of $POCl_3$ in acetonitrile yielded the title compound. The synthetic route for the synthesis of title compound is portrayed in **Scheme 1**. The title compound was characterized by FT-IR, ^{1}H NMR and ^{13}C NMR spectra. Further, pale yellow colored crystals suitable for X-ray diffraction analysis were grown by slow evaporation of a dilute solution of title compound in chloroform (m. p.136˚C - 138˚C) at room temperature.

2.2. Physical and Spectral Measurements

Melting point was determined in open capillary tubes on



Scheme 1. Synthetic route for the synthesis of title compound.

a melting point apparatus of Concord Instruments (P) Ltd., Bangalore and is uncorrected. The IR absorption spectrum was recorded on a Shimadzu FT-IR-8400S Spectrophotometer using KBr pellets and is reported as wave numbers (ν cm^{-1}). The ^{1}H NMR spectrum was determined on a Bruker AV400 II at 400 MHz. The ^{13}C NMR spectrum was recorded on Bruker DSX-300(S) AV-III 400(L) model at 100 MHz. All materials were purchased from commercial companies and are used directly. The solvents were dried by refluxing with appropriate drying agents and distilled before use.

2.3. Single-Crystal X-Ray Crystallography

Pale yellow colored crystals of the size of 0.30 × 0.20 × 0.20 mm was selected for data collection under a polarizing microscope and it was mounted on glass fiber for X-ray diffraction data collection. The high resolution X-ray diffraction data sets were collected on a Bruker SMART APEX2 CCD Diffractometer using Mo K_α radiation (λ = 0.71073 Å) at ambient temperature. The crystal-to-detector distance was fixed at 40 mm. The diffraction data have been scaled for absorption effect by the multi-scanning method. The total exposure time was 0.98 h. The frames were integrated with the Bruker SAINT Software package using a narrow-frame algorithm. The structure was solved and refined using the Bruker SHELXTL [12] Software Package, using the space group $Pna2_1$, with Z = 4 for the formula unit, $C_{20}H_{18}FNO$. The ORTEP, packing and planes diagrams are generated using the Mercury 3.1.

3. Results and Discussion

3.1. Crystal Structure

The integration of the crystal data of the title compound (E)-3-(3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl) acrylaldehyde using an orthorhombic unit cell yielded a total of 5558 reflections to a maximum θ angle of 23.92˚ (0.88 Å resolution), of which 2408 were independent (average redundancy 2.308, completeness = 99.5%, R_{int} = 2.25%, R_{sig} = 2.93%) and 2108 (87.54%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.4637(4) Å, b = 9.9386(3) Å, c = 13.0272(3) Å, volume = 1613.70(8) Å^3, are based upon the refinement of the XYZ-centroids of 1826 reflections above 20 σ(I) with 6.10˚ < 2θ < 47.84˚. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.978. The crystal data and structure refinement parameters are given in **Table 1**.

The final anisotropic full-matrix least-squares refinement on F^2 with 210 variables converged at R1 = 4.26%, for the observed data and wR2 = 8.48% for all data. The goodness-of-fit was 1.028. The largest peak in the final

Table 1. Crystal data and structure refinement.

Empirical formula	$C_{20}H_{18}FNO$
Formula weight	307.35
Temperature	296 K
Crystal size	0.30 × 0.20 × 0.20 mm
Crystal color	Pale yellow
Crystal system	Orthorhombic
Space group	$Pna2_1$
a	12.4637 (4) (Å)
b	9.9386 (3) (Å)
c	13.0272 (3) (Å)
α, β and γ	90˚, 90˚ and 90˚
Limiting indices	$-10 \le h \le 14$, $-11 \le k \le 11$, $-14 \le l \le 14$
Volume	1613.70 (8) (Å^3)
Z, Calculated density	4, 1.265 mg/m^3
Reflections collected/unique	5558/2408 [R(int) = 0.0225]
θ range for data collection and completeness	θ_{max} = 23.92˚, θ_{min} = 3.05˚ and 99.5%
Maximum and minimum transmission	0.972 and 0.951
Absorption correction	Semi-empirical from equivalents
Data/Restraints/Paramaeters	2408/2/211
Final R indices [I > 2σ(I)]	R1 = 0.0347, wR2 = 0.0804
R indices (all data)	R1 = 0.0426, wR2 = 0.0848
Absolute structure parameter	−2.3 (12)
Extinction coefficient	0.0071 (14)
Largest diff. peak and hole	0.151 and −0.105 e. Å^{-3}
Measurements	Bruker SMART APEX2 CCD Diffractometer
Refinement	Full-matrix leastsquares on F^2
Goodness-of-fit on F^2	1.028

difference electron density synthesis was 0.151 e. $Å^{-3}$ and the largest hole was −0.105 e. $Å^{-3}$ with an RMS deviation of 0.026 e. $Å^{-3}$. On the basis of the final model, the calculated density was 1.265 mg/m^3 and F (000), 648 e^-.

3.2. Molecular Skeleton

The structure of the compound consisted of butenal and fluorobenzene fragments that connected to N-isopropyl-indole moiety. The ORTEP diagram of the title compound is given in **Figure 1**. The 4-F-phenyl ring C4-C3 form dihedral angle with the mean plane of the nine membered indole ring system was 111.5 (3)˚ (**Figure 2**). The sum of the bond angles around N1 [359.9 (3)˚] indicated sp^2 hybridization [13]. The packing diagram (**Figure 3**) of the title molecule showed 4 molecules pack in a unit cell and no strong hydrogen bonds in the crystal structure were observed. However, weak inter molecular hydrogen bonds observed between C11H11···O1 by a distance of 2.692 Å are shown in **Figure 4**. All bond lengths and bond angles are in normal ranges and are given in **Table 2**. Atomic coordinates and equivalent isotropic displacement parameters are shown in **Table 3**. Anisotropic dis-placement parameters are shown in **Table 4**. Hydrogen coordinates and isotropic displacement parameters are shown in **Table 5**. Torsion angles are shown in **Table 6**.

3.3. Spectral Studies

3.3.1. FTIR Spectrum

The FT-IR spectrum of the title compound shows the strong characteristic absorption band at 1666.38 cm^{-1} due to aldehyde carbonyl stretching frequency. The shift in the band to lower wavenumber was due to the presence of α, β unsaturation. The band at 1610.45 cm^{-1} was observed due to C=C stretching.

3.3.2. ^{1}H NMR Spectrum

The ^{1}H NMR spectrum of the title compound showed two singlets at δ 1.64 and 1.66 ppm due to two methyl protons. The doublet at δ 9.61 ppm was attributed to aldehyde proton; it coupled with adjacent C8-CH protons with coupling constant of 7.6 Hz and the doublet at δ 7.95 ppm was accounted for vinylic proton with J value of 16 Hz. Further, C7 proton splits C8 proton signal into doublet (J = 16 Hz) which is split by C9 aldehyde proton into new doublets (J = 7.6 Hz) producing four-line spectrum (doublet of doublet) at δ 6.115 ppm. The signals appeared around δ 7.70 - 7.78 ppm were attributed to aromatic protons. ^{1}H NMR (400 MHz, DMSO-d6) δ ppm: 1.649 (s, 3H, C19-CH_3), 1.666 (s, 3H, C20-CH_3), 5.107 (m, 1H, C18-CH), 6.115 (dd, 1H, J = 16, 7.6 Hz, C8-CH), 7.959 (d, 1H, J = 16Hz, C7-CH), 9.619 (d, 1H, J = 7.6Hz, C9-CHO), 7.709 - 7.782 (m, 8H, Ar-H,).

3.3.3. ^{13}C NMR Spectrum

The ^{13}C NMR of the title compound exhibited a signal at δ 194.02 ppm for carbonyl carbon of the aldehyde group. The low intensity signal at δ 162.62 ppm was assigned to C1 carbon attached fluorine atom and the methyl carbons were observed at δ 21.37 ppm. The signal at δ 47.39 ppm was attributed to CH carbon of the isopropyl group. The peaks appeared between δ 112.60 - 160.20 ppm were assigned to aromatic and vinylic carbon atoms. ^{13}C NMR ($CDCl_3$, 100 MHz, δ ppm): 21.37 CH_3, 47.39 C18-CH, 162.62 C1-CF, 194.02 C9-CHO, 112, 115, 119, 120, 124, 127, 130, 132, 136, 141, 160 Ar-C.

4. Conclusion

The title compound, a key starting material for the syn-

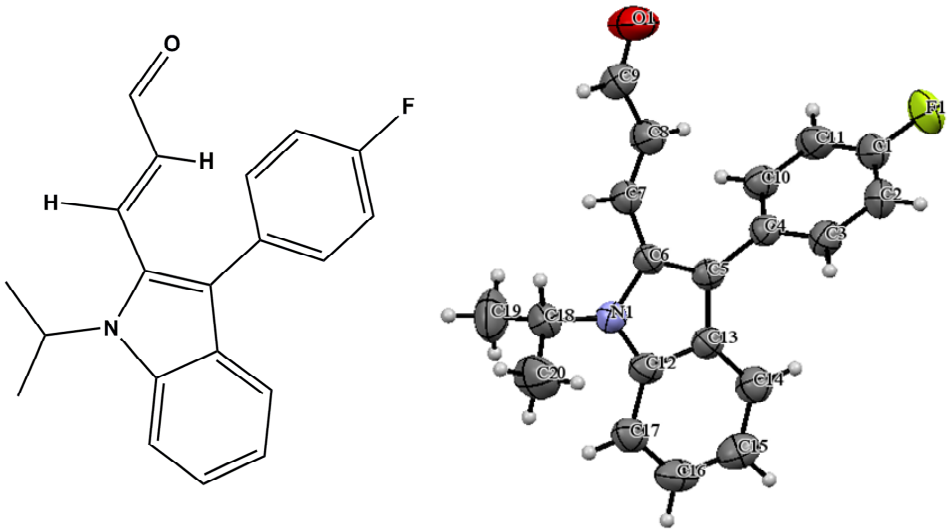


Figure 1. ORTEP diagram of the title molecule.

Table 2. Bond lengths [Å] and angles [˚].

Bond Lengths		Bond Angles	
F(1)-C(1)	1.363(3)	C(12)-N(1)-C(6)	108.34(18)
O(1)-C(9)	1.196(3)	C(12)-N(1)-C(18)	126.95(19)
N(1)-C(12)	1.381(3)	C(6)-N(1)-C(18)	124.66(19)
N(1)-C(6)	1.401(3)	C(11)-C(1)-C(2)	123.2(2)
N(1)-C(18)	1.477(3)	C(11)-C(1)-F(1)	118.8(3)
C(1)-C(11)	1.350(4)	C(2)-C(1)-F(1)	118.0(3)
C(1)-C(2)	1.363(4)	C(1)-C(2)-C(3)	117.7(3)
C(2)-C(3)	1.381(3)	C(1)-C(2)-H(2)	121.1
C(2)-H(2)	0.9300	C(3)-C(2)-H(2)	121.1
C(3)-C(4)	1.388(3)	C(2)-C(3)-C(4)	121.9(2)
C(3)-H(3)	0.9300	C(2)-C(3)-H(3)	119.1
C(4)-C(10)	1.389(3)	C(4)-C(3)-H(3)	119.1
C(4)-C(5)	1.475(3)	C(3)-C(4)-C(10)	117.7(2)
C(5)-C(6)	1.382(3)	C(3)-C(4)-C(5)	120.49(19)
C(5)-C(13)	1.414(3)	C(10)-C(4)-C(5)	121.7(2)
C(6)-C(7)	1.447(3)	C(6)-C(5)-C(13)	107.7(2)
C(7)-C(8)	1.295(3)	C(6)-C(5)-C(4)	128.8(2)
C(7)-H(7)	0.9300	C(13)-C(5)-C(4)	123.4(2)
C(8)-C(9)	1.429(3)	C(5)-C(6)-N(1)	108.57(19)
C(8)-H(8)	0.9300	C(5)-C(6)-C(7)	129.9(2)
C(9)-H(9)	0.9300	N(1)-C(6)-C(7)	121.5(2)
C(10)-C(11)	1.390(3)	C(8)-C(7)-C(6)	131.8(2)
C(10)-H(10)	0.9300	C(8)-C(7)-H(7)	114.1
C(11)-H(11)	0.9300	C(6)-C(7)-H(7)	114.1
C(12)-C(17)	1.396(3)	C(7)-C(8)-C(9)	122.8(2)
C(12)-C(13)	1.412(3)	C(7)-C(8)-H(8)	118.6
C(13)-C(14)	1.398(3)	C(9)-C(8)-H(8)	118.6
C(14)-C(15)	1.371(4)	O(1)-C(9)-C(8)	128.4(3)
C(14)-H(14)	0.9300	O(1)-C(9)-H(9)	115.8
C(15)-C(16)	1.399(4)	C(8)-C(9)-H(9)	115.8
C(15)-H(15)	0.9300	C(4)-C(10)-C(11)	120.8(2)
C(16)-C(17)	1.370(4)	C(4)-C(10)-H(10)	119.6
C(16)-H(16)	0.9300	C(11)-C(10)-H(10)	119.6
C(17)-H(17)	0.9300	C(1)-C(11)-C(10)	118.7(2)
C(18)-C(20)	1.485(4)	C(1)-C(11)-H(11)	120.7
C(18)-C(19)	1.502(4)	C(10)-C(11)-H(11)	120.7
C(18)-H(18)	0.9800	N(1)-C(12)-C(17)	131.6(2)
C(19)-H(19A)	0.9600	N(1)-C(12)-C(13)	107.92(19)
C(19)-H(19B)	0.9600	C(17)-C(12)-C(13)	120.5(2)
C(19)-H(19C)	0.9600	C(14)-C(13)-C(12)	119.9(2)
C(20)-H(20A)	0.9600	C(14)-C(13)-C(5)	132.7(2)
C(20)-H(20B)	0.9600	C(12)-C(13)-C(5)	107.4(2)
C(20)-H(20C)	0.9600	C(15)-C(14)-C(13)	119.1(2)

Continued

Bond Angles			
C(13)-C(14)-H(14)	120.4	C(15)-C(14)-H(14)	120.4
C(14)-C(15)-H(15)	119.9	C(14)-C(15)-C(16)	120.3(3)
C(17)-C(16)-C(15)	122.1(2)	C(16)-C(15)-H(15)	119.9
C(15)-C(16)-H(16)	118.9	C(17)-C(16)-H(16)	118.9
C(16)-C(17)-H(17)	121.0	C(16)-C(17)-C(12)	118.0(2)
N(1)-C(18)-C(20)	113.0(2)	C(12)-C(17)-H(17)	121.0
C(20)-C(18)-C(19)	115.4(2)	N(1)-C(18)-C(19)	110.1(2)
C(20)-C(18)-H(18)	105.8	N(1)-C(18)-H(18)	105.8
C(18)-C(19)-H(19A)	109.5	C(19)-C(18)-H(18)	105.8
H(19A)-C(19)-H(19B)	109.5	C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19C)	109.5	C(18)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5	H(19B)-C(19)-H(19C)	109.5
H(20A)-C(20)-H(20B)	109.5	C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20C)	109.5	C(18)-C(20)-H(20C)	109.5
		H(20B)-C(20)-H(20C)	109.5

Table 3. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	X	Y	Z	U(eq)
F(1)	6616(2)	1344(2)	10599(2)	100(1)
O(1)	8210(2)	7666(2)	11792(2)	93(1)
N(1)	4331(2)	8390(2)	9129(1)	48(1)
C(1)	6155(2)	2534(3)	10322(2)	63(1)
C(2)	6182(2)	2889(3)	9311(2)	63(1)
C(3)	5712(2)	4094(2)	9035(2)	53(1)
C(4)	5236(2)	4936(2)	9754(2)	45(1)
C(5)	4724(2)	6205(2)	9430(2)	45(1)
C(6)	5045(2)	7513(2)	9621(2)	45(1)
C(7)	5979(2)	8008(2)	10162(2)	51(1)
C(8)	6651(2)	7421(2)	10773(2)	61(1)
C(9)	7554(2)	8099(3)	11210(2)	58(1)
C(10)	5217(2)	4509(2)	10769(2)	54(1)
C(11)	5684(2)	3295(3)	11053(2)	63(1)
C(12)	3543(2)	7631(2)	8660(2)	48(1)
C(13)	3789(2)	6260(2)	8817(2)	46(1)
C(14)	3131(2)	5264(3)	8396(2)	60(1)
C(15)	2250(2)	5638(3)	7836(2)	68(1)
C(16)	2005(2)	7001(3)	7703(2)	67(1)
C(17)	2628(2)	8003(3)	8111(2)	57(1)
C(18)	4405(2)	9873(2)	9159(2)	60(1)
C(19)	3702(3)	10420(3)	9997(3)	98(1)
C(20)	4263(3)	10505(3)	8135(3)	94(1)

Table 4. Anisotropic displacement parameters (Å × 10^3). The anisotropic displacement factor exponent takes the form: $-2\pi^2\left[h^2a^{*2}U_{11}+\cdots+2hka^{*}b^{*}U_{12}\right]$.

	U11	U22	U33	U23	U13	U12
F(1)	137(2)	45(1)	118(2)	6(1)	−40(1)	20(1)
O(1)	91(2)	97(2)	91(2)	14(1)	−42(1)	−12(1)
N(1)	58(1)	44(1)	44(1)	−3(1)	−6(1)	6(1)
C(1)	75(2)	38(2)	75(2)	2(1)	−20(2)	1(1)
C(2)	74(2)	47(2)	69(2)	−9(1)	−4(1)	6(1)
C(3)	60(1)	50(1)	48(1)	−2(1)	2(1)	−3(1)
C(4)	49(1)	42(1)	43(1)	−1(1)	−2(1)	−3(1)
C(5)	50(1)	47(1)	37(1)	2(1)	2(1)	1(1)
C(6)	52(1)	46(1)	36(1)	1(1)	1(1)	8(1)
C(7)	58(1)	43(1)	51(1)	−1(1)	−3(1)	2(1)
C(8)	71(2)	49(2)	63(2)	7(1)	−14(2)	−3(1)
C(9)	62(2)	62(2)	51(2)	−4(1)	−4(1)	−3(1)
C(10)	64(2)	53(2)	44(1)	0(1)	−3(1)	−1(1)
C(11)	83(2)	53(2)	54(1)	13(1)	−16(1)	−8(1)
C(12)	49(1)	59(2)	37(1)	0(1)	1(1)	6(1)
C(13)	50(1)	51(2)	39(1)	−1(1)	2(1)	2(1)
C(14)	63(2)	58(2)	59(2)	2(1)	−2(1)	−4(1)
C(15)	62(2)	80(2)	63(2)	−3(2)	−10(1)	−11(1)
C(16)	53(2)	91(2)	57(2)	4(2)	−9(1)	6(1)
C(17)	58(2)	66(2)	48(1)	0(1)	−1(1)	10(1)
C(18)	67(2)	48(2)	66(2)	−2(1)	−10(1)	9(1)
C(19)	103(2)	74(2)	118(3)	−35(2)	14(2)	16(2)
C(20)	113(3)	66(2)	101(3)	30(2)	−23(2)	−9(2)

Table 5. Hydrogen coordinates (×10^4) and isotropic displacement parameters (Å^2 × 10^3).

	X	Y	Z	U(eq)
H(2)	6505	2338	8825	76
H(3)	5714	4349	8348	63
H(7)	6123	8914	10049	76
H(8)	6542	6520	10935	73
H(9)	7642	8993	11016	70
H(10)	4888	5041	11264	64
H(11)	5673	3012	11734	76
H(14)	3290	4358	8494	72
H(15)	1812	4984	7543	82
H(16)	1399	7234	7326	81
H(17)	2447	8904	8025	69
H(18)	5143	10077	9367	72
H(19A)	3888	10002	10637	147
H(19B)	2964	10232	9839	147
H(19C)	3803	11375	10050	147
H(20A)	3512	10544	7972	140
H(20B)	4630	9979	7626	140
H(20C)	4553	11399	8146	140

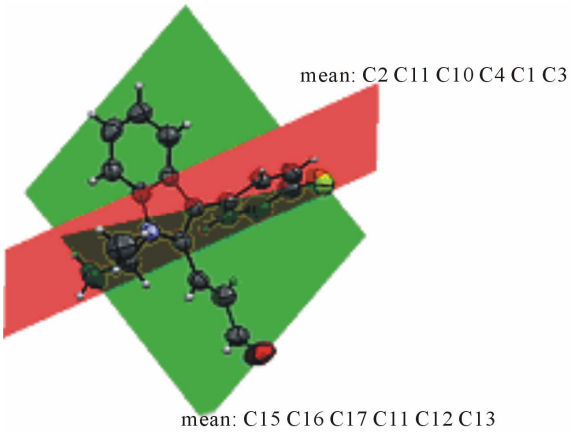


Figure 2. Dihedral angle formed between indole plane and benzene plane.

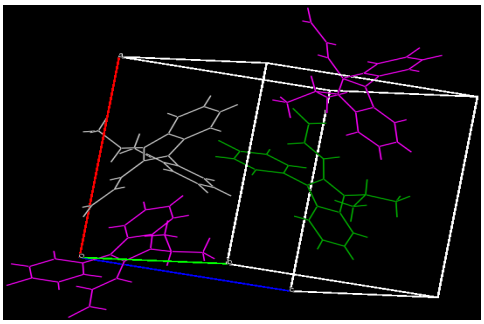


Figure 3. Packing diagram of title compound, ab Plane, colored by symmetry operation.

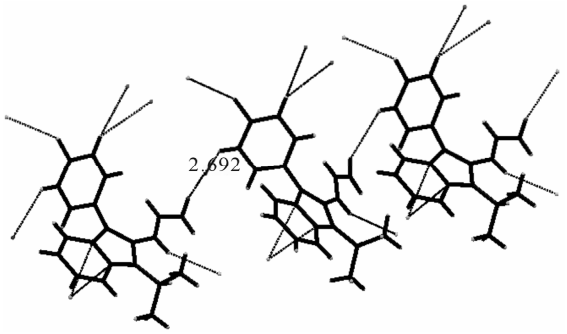


Figure 4. Diagram showing inter molecular weak Hydrogen bonding.

Table 6. Torsion angles [˚].

C(11)-C(1)-C(2)-C(3)	0.8(4)
F(1)-C(1)-C(2)-C(3)	179.9(2)
C(1)-C(2)-C(3)-C(4)	0.7(4)
C(2)-C(3)-C(4)-C(10)	−1.9(4)
C(2)-C(3)-C(4)-C(5)	−178.9(2)
C(3)-C(4)-C(5)-C(6)	−111.5(3)
C(10)-C(4)-C(5)-C(6)	71.6(3)
C(3)-C(4)-C(5)-C(13)	66.7(3)
C(10)-C(4)-C(5)-C(13)	−110.2(3)
C(13)-C(5)-C(6)-N(1)	−0.6(2)
C(4)-C(5)-C(6)-N(1)	177.8(2)
C(13)-C(5)-C(6)-C(7)	−176.5(2)
C(4)-C(5)-C(6)-C(7)	1.9(4)
C(12)-N(1)-C(6)-C(5)	2.1(2)
C(18)-N(1)-C(6)-C(5)	179.6(2)
C(12)-N(1)-C(6)-C(7)	178.39(19)
C(18)-N(1)-C(6)-C(7)	−4.1(3)
C(5)-C(6)-C(7)-C(8)	−15.2(4)
N(1)-C(6)-C(7)-C(8)	169.3(3)
C(6)-C(7)-C(8)-C(9)	178.1(2)
C(7)-C(8)-C(9)-O(1)	178.6(3)
C(3)-C(4)-C(10)-C(11)	1.6(4)
C(5)-C(4)-C(10)-C(11)	178.6(2)
C(2)-C(1)-C(11)-C(10)	−1.0(4)
F(1)-C(1)-C(11)-C(10)	179.9(2)
C(4)-C(10)-C(11)-C(1)	−0.2(4)
C(6)-N(1)-C(12)-C(17)	177.1(2)
C(18)-N(1)-C(12)-C(17)	−0.4(4)
C(6)-N(1)-C(12)-C(13)	−2.7(2)
C(18)-N(1)-C(12)-C(13)	179.8(2)
N(1)-C(12)-C(13)-C(14)	−178.29(19)
C(17)-C(12)-C(13)-C(14)	1.9(3)
N(1)-C(12)-C(13)-C(5)	2.4(2)

Continued

C(17)-C(12)-C(13)-C(5)	−177.5(2)
C(6)-C(5)-C(13)-C(14)	179.7(2)
C(4)-C(5)-C(13)-C(14)	1.2(4)
C(6)-C(5)-C(13)-C(12)	−1.1(2)
C(4)-C(5)-C(13)-C(12)	−179.62(19)
C(12)-C(13)-C(14)-C(15)	−0.2(3)
C(5)-C(13)-C(14)-C(15)	178.9(2)
C(13)-C(14)-C(15)-C(16)	−1.0(4)
C(14)-C(15)-C(16)-C(17)	0.6(4)
C(15)-C(16)-C(17)-C(12)	1.1(4)
N(1)-C(12)-C(17)-C(16)	178.0(2)
C(13)-C(12)-C(17)-C(16)	−2.3(3)
C(12)-N(1)-C(18)-C(20)	−48.7(3)
C(6)-N(1)-C(18)-C(20)	134.3(2)
C(12)-N(1)-C(18)-C(19)	82.0(3)
C(6)-N(1)-C(18)-C(19)	−95.0(3)

thesis of fluvastatin was synthesized, its spectral data were discussed and single crystals were grown. The crystal parameters were evaluated. Bond lengths and bond angles are in normal ranges. No classical hydrogen bonding was observed. The 4-F-phenyl ring C4-C3 form dihedral angle with the mean plane of the nine membered indole ring system was 111.5 (3)˚.

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