J. Chosun Natural Sci.
Vol. 7, No. 3 (2014) pp. 149 – 158
http://dx.doi.org/10.13160/ricns.2014.7.3.149

Crystal and Molecular Structure of 12-(2-Methoxyphenyl)-9-[(4-methylbenzene)sulfonyl]-22-oxo-13,21-dioxa-9-azapentacyclo [12.8.0.0^{2,11}.0^{3,8}.0^{15,20}]docosa-1(14),3,5,7,15(20),16,18-heptaene-11-carbonitrile

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Abstract

The crystal structure of the title compounds with both coumarin and sulfonamide moieties were examined. These two groups have very special for their pharmaceutical and medicinal properties have been determined from single crystal X-ray diffraction data. In the title compound crystallizes in the monoclinic space group $P2_1/c$ with unit cell dimension a= 8.5775(4)Å, b= 24.9943(13)Å and c=13.7319(7)Å [alpha & gamma=90° beta= 103.558(2)°]. In the structure The S1 atom shows a distorted tetrahedral geometry, with O1—S1—O2 [121.08 (1)°] and N1-S1-C5 [105.85 (1)°] angles deviating from ideal tetrahedral values are attributed to the Thrope-Ingold effect. The sum of bond angles around N1 (354.9°) indicates that N1 is in sp^2 hybridization. The Pyridine ring adopts boat conformation and pyran rings adopt a sofa conformation. Crystal structure is stabilized by C-H…O intra molecular hydrogen bond interactions.

Key words: Pyrone, Pyran, Coumarin, Sulfonamide, Single Crystal Structure, X-ray Diffraction

1. Introduction

In our previous study, crystal structure of one of the coumarin derivatives have been reported[1]. Here we have analyzed a compound with both coumarin and sulfonamide moieties were examined. These two groups have very special for their pharmaceutical and medicinal properties. Hence, a practical method for the preparation of such compounds is of great interest in synthetic organic chemistry. Coumarin derivatives alone are known to be an interesting class of natural or synthetic compounds, whose biological activity varies according to the substitutes on the benzopyran ring and their antibacterial, antifungal, antitumor, anti-HIV, and anti-inflammatory. These derivatives show strong activity against cancer cell lines[2] and exhibit monoamine oxidase inhibitory activity[3]. Antiulcer activity of some naturally occurring pyranocoumarins has been reported[4]. It also shows specific inhibitory activity against Hepatitis B virus, anti-filarial[5], cytotoxic activites[6] and Mycobacterium tuberculosis[7]. One of the natural source coumarin derivatives named, Chalepin, inhibits the enzyme glyceraldehyde-3-phosphate dehydrogenase of Trypanosoma cruzi and its complex structure has deposited in Protein Data Bank (1K3T)[8] and also sulfonamide based derivatives has wide range biological activity and many of the sulfo based drugs are currently available in the market. In view of this biological importance, X-ray diffraction studies have been undertaken for one coumarin-sulonamide derivatives and here we report the crystal structure of the title compound.

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(Received : June 14, 2014, Revised : September 23, 2014, Accepted : September 25, 2014)

2. Experimental Section

2.1. Material and Methods

With the collaboration of Organic Chemistry Department at University of Madras, we obtained the title compound and crystallized by simple solvent slow evaporation method. Three rounds of crystallization trials, diffraction crystals.

The diffraction quality crystals after screening its size and stability, X-ray diffraction data collection was done

at University of Madras-Technology Business Incubator facility. The data was reduced with appropriate corrections at the facility and the error free data was taken for structure determination.

Using WinGx suite, structure determination was done using SHELXS97 with Direct Methods protocols. After manual inspections and corrections, Isotropic refinement followed by anisotropic refinements was carried out. With the satisfied model (agreeable R factor, Goodness of Fit and other) hydrogen atoms were geometrically fixed and after the final refinement the R factor is 4.1%.

2.2. Synthesis of Title Compound

A well grounded mixture of (2Z)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfonamido] methyl}-3-(2-methoxyphenyl)prop-2-enenitrile (0.45 g, 1 mmol) and 4-hydroxy-2*H*-chromen-2-one, (0.16 g, 1 mmol) was placed in a round bottom flask and melted at 200°C for 1 h. After completion of the reaction as indicated by TLC, the crude product was washed with 5 mL of ethylacetate and hexane mixture (1:49 ratio) which successfully provided the pure product as colorless solid in 94% yield. Since the compound has not yield the diffraction quality crystals initially, the compound has been recrystallized with ethyl acetate by slow evaporation method to get better quality single crystals.

2.3. X-Ray Crystallography

For the crystal structure determination, the single crystal of the compound $C_{34}H_{26}N_2O_6S$ was used for data collection on a Bruker Kappa APEXII CCD diffractometer[9]. The MoK″ radiation of wavelength, (# = 0.71073 Å) and multi-scan technique for absorption correction were used for data collection. The lattice parameters were determined by the least-squares methods on the basis of all reflections with F2>2$ (F2). The structures were solved by direct methods using SHELXS-97 and refined by a full-matrix least-squares procedure using the program SHELXL-97[10,11]. H atoms were positioned geometrically and refined using a riding model, fixing the aromatic C-H distances at 0.93 Å [Uiso(H) = 1.2 Ueq (C)]. The softwares used for Molecular graphics are ORTEP-3 for Windows[12] and PLATON[13]. The software used to prepare material for publication is WinGX publication routines[14]. Experimental data are listed in Table 1. CCDC reference number: 902984. Fig. 1 shows schematic diagram of the molecule and molecular structure of the title compound along with the atom numbering scheme is depicted in Fig. 2 and a packing

Table 1. Crystal Data and Structure Refinement

Empirical formula	$C_{34}H_{26}N_2O_6S$
Formula weight	420.41
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 8.577 (4) (8) Å
	b = 24.994 (13) Å β = 98.113(2)°
	c = 13.731 (7) Å
Volume	2861.9(2) $Å^3$
Z, Calculated density	4, 1.371 Mg/m^3
Absorption coefficient	0.164 mm^{-1}
F(000)	1232
Crystal size	0.30×0.30×0.25 mm
θ range for data collection	1.63 to 25.0°
Limiting indices	-10<=h<=10, -29<=k<=29, -16<=l<=16
Reflections collected / unique	25474 / 5039 [Rint = 0.034]
Completeness to θ = 25.00	Completeness to θ = 25.00, 100%
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	5039 / 0 / 391
Goodness-of-fit on F2	1.06
Final R indices [I>2σ(I)]	R1 = 0.0410, wR2 = 0.0952
R indices (all data)	R1 = 0.0677, wR2 = 0.1208
Largest diff. peak and hole	-0.339 and 0.35 $e.Å^{-3}$

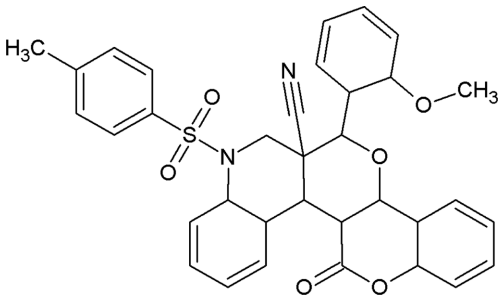

Fig. 1. Schematic diagram of the molecule.

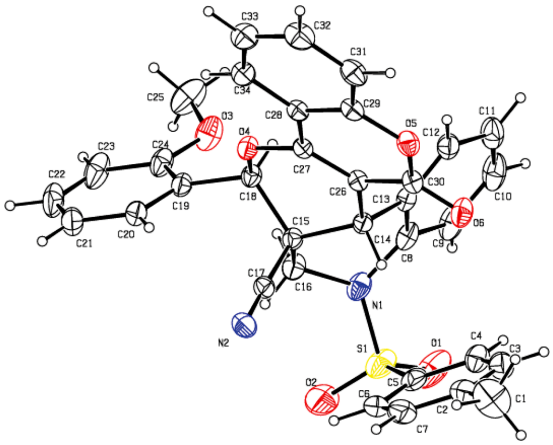

Fig. 2. Displacement ellipsoids are drawn at the 30% probability level.

diagram is shown in Fig. 3. Table 1 shows the crystal data and crystal refinement. Table 2 gives the atomic coordinates, Table 3 describes the bond lengths and

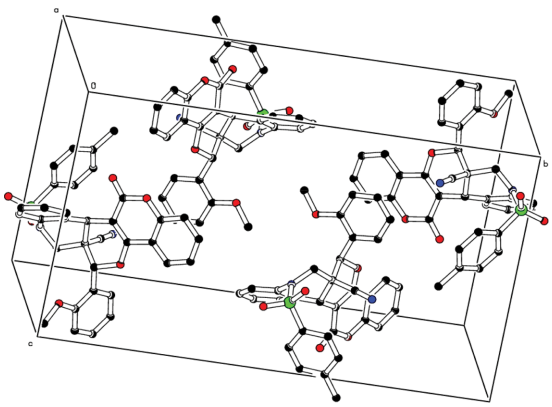

Fig. 3. Crystal packing of the title compound, H atoms have been omitted for clarity.

angles; Table 4 shows anisotropic displacement parameters and Table 5 shows the torsion angles.

3. Results and Discussion

Title compound crystallizes in the monoclinic centrosymmetric space group $P2_1/c$ with Z = 4. The structure of the compound consists of coumarine, pyran and sulfonamide fragments whose rings are connected to one another. All the three rings exhibit coplanarity with one another. The coumarin ring system adopts sofa/envelop conformation observed from previous deports in jagadeesan[15].

The molecular structure of the title compound is shown in Fig. 2.The S1 atom shows a distorted tetrahedral geometry, with O1—S1—O2 [121.08(1)°] and

Table 2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0450 (5)	0.16531 (16)	0.4418 (3)	0.1310 (14)
H1A	1.1209	0.1533	0.4051	0.196*
H1B	1.0711	0.2011	0.4651	0.196*
H1C	0.9391	0.1647	0.3989	0.196*
C2	1.0511 (3)	0.12913 (12)	0.5295 (2)	0.0782 (8)
C3	0.9784 (3)	0.07988 (11)	0.5169 (2)	0.0747 (7)
H3	0.9260	0.0690	0.4528	0.090*
C4	0.9810 (3)	0.04651 (11)	0.5958 (2)	0.0732 (7)
H4	0.9305	0.0134	0.5855	0.088*
C5	1.0598 (3)	0.06246 (11)	0.6915 (2)	0.0690 (7)
C6	1.1336 (3)	0.11210 (13)	0.7052 (2)	0.0794 (8)
H6	1.1873	0.1232	0.7690	0.095*
C7	1.1270 (3)	0.14457 (13)	0.6245 (3)	0.0838 (9)

Table 2. Continued

	x	y	z	U_{iso}*/U_{eq}
H7	1.1753	0.1781	0.6343	0.101*
C8	0.7270 (3)	0.02033 (9)	0.74194 (18)	0.0612 (6)
C9	0.6824 (5)	-0.03248 (10)	0.7208 (2)	0.0834 (9)
H9	0.7485	-0.0601	0.7516	0.100*
C10	0.5409 (5)	-0.04367 (12)	0.6546 (3)	0.0925 (10)
H10	0.5125	-0.0790	0.6383	0.111*
C11	0.4406 (4)	-0.00317 (12)	0.6119 (2)	0.0821 (9)
H11	0.3426	-0.0113	0.5688	0.099*
C12	0.4839 (3)	0.04987 (10)	0.63236 (18)	0.0620 (6)
H12	0.4149	0.0772	0.6032	0.074*
C13	0.6294 (3)	0.06200 (8)	0.69600 (16)	0.0509 (5)
C14	0.6981 (2)	0.11800 (8)	0.71315 (15)	0.0445 (5)
H14	0.7884	0.1193	0.6807	0.053*
C15	0.7695 (2)	0.12881 (8)	0.82615 (15)	0.0464 (5)
C16	0.8463 (3)	0.07746 (9)	0.88181 (17)	0.0609 (6)
H16A	0.9493	0.0868	0.9250	0.073*
H16B	0.7781	0.0646	0.9241	0.073*
C17	0.8916 (3)	0.17106 (9)	0.83299 (16)	0.0511 (5)
C18	0.6349 (3)	0.14786 (8)	0.87510 (15)	0.0468 (5)
H18	0.5536	0.1196	0.8671	0.056*
C19	0.6890 (3)	0.16109 (9)	0.98473 (16)	0.0531 (6)
C20	0.7714 (3)	0.20786 (11)	1.01564 (19)	0.0669 (7)
H20	0.7939	0.2311	0.9679	0.080*
C21	0.8207 (3)	0.22086 (14)	1.1150 (2)	0.0873 (9)
H21	0.8770	0.2524	1.1346	0.105*
C22	0.7861 (4)	0.18710 (17)	1.1844 (2)	0.1009 (12)
H22	0.8192	0.1959	1.2519	0.121*
C23	0.7031 (4)	0.14016 (14)	1.1572 (2)	0.0952 (11)
H23	0.6811	0.1175	1.2059	0.114*
C24	0.6526 (3)	0.12701 (11)	1.05632 (18)	0.0659 (7)
C25	0.4965 (5)	0.05241 (13)	1.0873 (3)	0.1072 (12)
H25A	0.5789	0.0346	1.1358	0.161*
H25B	0.4240	0.0264	1.0502	0.161*
H25C	0.4387	0.0762	1.1210	0.161*
C26	0.5891 (2)	0.16319 (8)	0.66957 (15)	0.0434 (5)
C27	0.5316 (2)	0.19839 (8)	0.72692 (15)	0.0430 (5)
C28	0.4345 (2)	0.24345 (8)	0.68447 (16)	0.0460 (5)
C29	0.4030 (2)	0.24925 (9)	0.58148 (17)	0.0515 (5)
C30	0.5616 (3)	0.17230 (9)	0.56304 (16)	0.0515 (5)
C31	0.3055 (3)	0.28961 (10)	0.5328 (2)	0.0675 (7)
H31	0.2863	0.2934	0.4636	0.081*
C32	0.2377 (3)	0.32394 (10)	0.5889 (2)	0.0762 (8)
H32	0.1705	0.3511	0.5572	0.091*
C33	0.2674 (3)	0.31893 (10)	0.6918 (2)	0.0712 (7)

Table 2. Continued

	x	*y*	*z*	U_{iso}*/U_{eq}
H33	0.2202	0.3426	0.7286	0.085*
C34	0.3661 (3)	0.27931 (9)	0.73972 (19)	0.0574 (6)
H34	0.3874	0.2764	0.8091	0.069*
N1	0.8698 (3)	0.03415 (8)	0.81495 (15)	0.0655 (6)
N2	0.9867 (2)	0.20309 (9)	0.83530 (15)	0.0691 (6)
O1	1.0452 (3)	-0.03209 (9)	0.76159 (19)	0.1225 (9)
O2	1.1606 (3)	0.04034 (11)	0.88015 (17)	0.1223 (9)
O3	0.5677 (3)	0.08227 (8)	1.02022 (14)	0.0860 (6)
O4	0.55957 (17)	0.19563 (6)	0.82748 (10)	0.0506 (4)
O5	0.46350 (18)	0.21417 (6)	0.52269 (11)	0.0572 (4)
O6	0.6165 (2)	0.14593 (7)	0.50601 (12)	0.0704 (5)
S1	1.04720 (10)	0.02222 (3)	0.79339 (6)	0.0901 (3)

Table 3. Bond lengths [Å] and angles [°]

C1—C2	1.498 (4)	C18—C19	1.505 (3)
C1—H1A	0.9600	C18—H18	0.9800
C1—H1B	0.9600	C19—C20	1.380 (3)
C1—H1C	0.9600	C19—C24	1.391 (3)
C2—C7	1.370 (4)	C20—C21	1.369 (4)
C2—C3	1.372 (4)	C20—H20	0.9300
C3—C4	1.363 (4)	C21—C22	1.356 (5)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.389 (4)	C22—C23	1.378 (5)
C4—H4	0.9300	C22—H22	0.9300
C5—C6	1.386 (4)	C23—C24	1.390 (4)
C5—S1	1.747 (3)	C23—H23	0.9300
C6—C7	1.364 (4)	C24—O3	1.363 (3)
C6—H6	0.9300	C25—O3	1.429 (3)
C7—H7	0.9300	C25—H25A	0.9600
C8—C9	1.386 (4)	C25—H25B	0.9600
C8—C13	1.391 (3)	C25—H25C	0.9600
C8—N1	1.432 (3)	C26—C27	1.349 (3)
C9—C10	1.364 (4)	C26—C30	1.444 (3)
C9—H9	0.9300	C27—O4	1.347 (2)
C10—C11	1.369 (4)	C27—C28	1.440 (3)
C10—H10	0.9300	C28—C29	1.384 (3)
C11—C12	1.388 (4)	C28—C34	1.390 (3)
C11—H11	0.9300	C29—O5	1.374 (3)
C12—C13	1.379 (3)	C29—C31	1.379 (3)
C12—H12	0.9300	C30—O6	1.201 (3)
C13—C14	1.516 (3)	C30—O5	1.375 (3)
C14—C26	1.499 (3)	C31—C32	1.371 (4)
C14—C15	1.553 (3)	C31—H31	0.9300

Table 3. Continued

C14—H14	0.9800	C32—C33	1.382 (4)
C15—C17	1.474 (3)	C32—H32	0.9300
C15—C18	1.542 (3)	C33—C34	1.367 (3)
C15—C16	1.558 (3)	C33—H33	0.9300
C16—N1	1.464 (3)	C34—H34	0.9300
C16—H16A	0.9700	N1—S1	1.644 (2)
C16—H16B	0.9700	O1—S1	1.425 (2)
C17—N2	1.138 (3)	O2—S1	1.424 (2)
C18—O4	1.439 (2)		
	Bond Angle		
C2—C1—H1A	109.5	C19—C18—H18	108.3
C2—C1—H1B	109.5	C15—C18—H18	108.3
H1A—C1—H1B	109.5	C20—C19—C24	119.0 (2)
C2—C1—H1C	109.5	C20—C19—C18	120.6 (2)
H1A—C1—H1C	109.5	C24—C19—C18	120.3 (2)
H1B—C1—H1C	109.5	C21—C20—C19	121.6 (3)
C7—C2—C3	118.3 (3)	C21—C20—H20	119.2
C7—C2—C1	121.0 (3)	C19—C20—H20	119.2
C3—C2—C1	120.7 (3)	C22—C21—C20	119.0 (3)
C4—C3—C2	121.7 (3)	C22—C21—H21	120.5
C4—C3—H3	119.1	C20—C21—H21	120.5
C2—C3—H3	119.1	C21—C22—C23	121.6 (3)
C3—C4—C5	119.4 (3)	C21—C22—H22	119.2
C3—C4—H4	120.3	C23—C22—H22	119.2
C5—C4—H4	120.3	C22—C23—C24	119.5 (3)
C6—C5—C4	119.4 (3)	C22—C23—H23	120.3
C6—C5—S1	121.2 (2)	C24—C23—H23	120.3
C4—C5—S1	119.0 (2)	O3—C24—C23	124.9 (3)
C7—C6—C5	119.4 (3)	O3—C24—C19	115.8 (2)
C7—C6—H6	120.3	C23—C24—C19	119.4 (3)
C5—C6—H6	120.3	O3—C25—H25A	109.5
C6—C7—C2	121.7 (3)	O3—C25—H25B	109.5
C6—C7—H7	119.1	H25A—C25—H25B	109.5
C2—C7—H7	119.1	O3—C25—H25C	109.5
C9—C8—C13	120.7 (3)	H25A—C25—H25C	109.5
C9—C8—N1	121.7 (2)	H25B—C25—H25C	109.5
C13—C8—N1	117.5 (2)	C27—C26—C30	119.55 (19)
C10—C9—C8	119.6 (3)	C27—C26—C14	122.54 (18)
C10—C9—H9	120.2	C30—C26—C14	117.50 (18)
C8—C9—H9	120.2	O4—C27—C26	124.29 (18)
C9—C10—C11	120.4 (3)	O4—C27—C28	113.72 (17)
C9—C10—H10	119.8	C26—C27—C28	121.98 (19)
C11—C10—H10	119.8	C29—C28—C34	118.9 (2)
C10—C11—C12	120.5 (3)	C29—C28—C27	116.86 (19)
C10—C11—H11	119.7	C34—C28—C27	124.2 (2)

Table 3. Continued

C12—C11—H11	119.7	O5—C29—C31	116.8 (2)
C13—C12—C11	119.9 (3)	O5—C29—C28	121.56 (19)
C13—C12—H12	120.1	C31—C29—C28	121.6 (2)
C11—C12—H12	120.1	O6—C30—O5	116.8 (2)
C12—C13—C8	118.8 (2)	O6—C30—C26	125.3 (2)
C12—C13—C14	124.2 (2)	O5—C30—C26	117.86 (19)
C8—C13—C14	116.8 (2)	C32—C31—C29	118.3 (2)
C26—C14—C13	116.77 (17)	C32—C31—H31	120.9
C26—C14—C15	109.32 (16)	C29—C31—H31	120.9
C13—C14—C15	111.34 (17)	C31—C32—C33	121.2 (2)
C26—C14—H14	106.2	C31—C32—H32	119.4
C13—C14—H14	106.2	C33—C32—H32	119.4
C15—C14—H14	106.2	C34—C33—C32	120.2 (3)
C17—C15—C18	110.14 (17)	C34—C33—H33	119.9
C17—C15—C14	107.21 (17)	C32—C33—H33	119.9
C18—C15—C14	109.23 (16)	C33—C34—C28	119.8 (2)
C17—C15—C16	110.28 (18)	C33—C34—H34	120.1
C18—C15—C16	108.31 (17)	C28—C34—H34	120.1
C14—C15—C16	111.67 (17)	C8—N1—C16	113.37 (19)
N1—C16—C15	113.95 (18)	C8—N1—S1	120.42 (16)
N1—C16—H16A	108.8	C16—N1—S1	121.10 (18)
C15—C16—H16A	108.8	C24—O3—C25	117.8 (2)
N1—C16—H16B	108.8	C27—O4—C18	117.48 (15)
C15—C16—H16B	108.8	C29—O5—C30	121.93 (17)
H16A—C16—H16B	107.7	O2—S1—O1	121.08 (16)
N2—C17—C15	177.7 (2)	O2—S1—N1	105.74 (13)
O4—C18—C19	105.82 (16)	O1—S1—N1	106.42 (14)
O4—C18—C15	111.13 (16)	O2—S1—C5	109.19 (16)
C19—C18—C15	114.65 (17)	O1—S1—C5	107.56 (14)
O4—C18—H18	108.3	N1—S1—C5	105.86 (11)

Table 4. Anisotropic displacement parameters

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.148 (4)	0.118 (3)	0.120 (3)	-0.025 (3)	0.017 (3)	0.029 (3)
C2	0.0622 (16)	0.079 (2)	0.092 (2)	-0.0028 (14)	0.0163 (15)	-0.0014 (17)
C3	0.0764 (18)	0.0749 (19)	0.0710 (18)	0.0009 (15)	0.0135 (14)	-0.0092 (15)
C4	0.0818 (18)	0.0592 (16)	0.081 (2)	0.0063 (14)	0.0231 (15)	-0.0138 (15)
C5	0.0573 (14)	0.0797 (19)	0.0724 (17)	0.0232 (14)	0.0201 (13)	-0.0074 (14)
C6	0.0441 (14)	0.107 (2)	0.087 (2)	-0.0022 (15)	0.0136 (13)	-0.0297 (19)
C7	0.0614 (17)	0.089 (2)	0.103 (2)	-0.0183 (15)	0.0247 (17)	-0.0135 (19)
C8	0.0874 (18)	0.0473 (14)	0.0567 (14)	0.0087 (12)	0.0328 (13)	-0.0017 (11)
C9	0.141 (3)	0.0453 (15)	0.0750 (19)	0.0058 (17)	0.047 (2)	0.0000 (14)
C10	0.157 (3)	0.0539 (18)	0.080 (2)	-0.030 (2)	0.054 (2)	-0.0165 (16)
C11	0.107 (2)	0.077 (2)	0.0692 (18)	-0.0364 (18)	0.0333 (17)	-0.0191 (16)

Table 4. Continued

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C12	0.0712 (16)	0.0604 (15)	0.0584 (15)	-0.0126 (12)	0.0234 (13)	-0.0111 (12)
C13	0.0652 (14)	0.0453 (12)	0.0467 (12)	-0.0021 (11)	0.0222 (11)	-0.0057 (10)
C14	0.0470 (11)	0.0447 (12)	0.0426 (12)	0.0020 (9)	0.0119 (9)	-0.0034 (9)
C15	0.0501 (12)	0.0459 (12)	0.0422 (12)	0.0059 (10)	0.0087 (9)	-0.0008 (9)
C16	0.0732 (15)	0.0577 (14)	0.0502 (13)	0.0189 (12)	0.0112 (12)	0.0045 (11)
C17	0.0483 (13)	0.0603 (14)	0.0413 (12)	0.0079 (11)	0.0034 (10)	-0.0027 (10)
C18	0.0534 (12)	0.0455 (12)	0.0412 (11)	0.0059 (10)	0.0107 (10)	0.0010 (9)
C19	0.0571 (13)	0.0597 (14)	0.0409 (12)	0.0153 (11)	0.0083 (10)	-0.0030 (11)
C20	0.0630 (15)	0.0762 (18)	0.0602 (16)	0.0066 (13)	0.0120 (12)	-0.0207 (13)
C21	0.0776 (19)	0.107 (2)	0.0679 (19)	0.0203 (17)	-0.0013 (15)	-0.0336 (19)
C22	0.115 (3)	0.123 (3)	0.0495 (18)	0.055 (2)	-0.0114 (17)	-0.025 (2)
C23	0.140 (3)	0.100 (2)	0.0449 (16)	0.057 (2)	0.0202 (17)	0.0125 (16)
C24	0.0867 (18)	0.0660 (17)	0.0462 (14)	0.0268 (14)	0.0178 (13)	0.0052 (12)
C25	0.152 (3)	0.088 (2)	0.105 (3)	0.026 (2)	0.077 (2)	0.0365 (19)
C26	0.0439 (11)	0.0428 (11)	0.0415 (11)	-0.0020 (9)	0.0062 (9)	-0.0022 (9)
C27	0.0408 (10)	0.0456 (12)	0.0402 (11)	-0.0042 (9)	0.0049 (9)	-0.0007 (9)
C28	0.0424 (11)	0.0422 (12)	0.0502 (13)	-0.0021 (9)	0.0045 (9)	0.0002 (10)
C29	0.0461 (12)	0.0477 (13)	0.0556 (14)	-0.0046 (10)	0.0020 (10)	0.0019 (11)
C30	0.0549 (13)	0.0520 (13)	0.0446 (13)	-0.0036 (11)	0.0055 (10)	-0.0024 (11)
C31	0.0651 (15)	0.0634 (16)	0.0632 (16)	0.0019 (13)	-0.0069 (13)	0.0109 (13)
C32	0.0695 (17)	0.0575 (16)	0.091 (2)	0.0136 (13)	-0.0021 (15)	0.0143 (15)
C33	0.0705 (16)	0.0528 (15)	0.087 (2)	0.0133 (12)	0.0114 (15)	0.0013 (14)
C34	0.0589 (14)	0.0486 (13)	0.0628 (15)	0.0038 (11)	0.0106 (11)	0.0000 (11)
N1	0.0831 (14)	0.0557 (12)	0.0596 (12)	0.0242 (11)	0.0203 (11)	0.0031 (10)
N2	0.0589 (12)	0.0822 (15)	0.0626 (13)	-0.0102 (12)	0.0070 (10)	-0.0067 (11)
O1	0.165 (2)	0.0829 (15)	0.135 (2)	0.0746 (15)	0.0671 (18)	0.0222 (14)
O2	0.0911 (15)	0.183 (3)	0.0809 (15)	0.0630 (16)	-0.0032 (12)	0.0127 (15)
O3	0.1329 (17)	0.0704 (12)	0.0672 (12)	0.0013 (12)	0.0486 (12)	0.0125 (10)
O4	0.0584 (9)	0.0513 (9)	0.0414 (8)	0.0124 (7)	0.0103 (7)	0.0000 (7)
O5	0.0625 (9)	0.0607 (10)	0.0430 (8)	0.0029 (8)	0.0014 (7)	0.0040 (7)
O6	0.0914 (13)	0.0745 (12)	0.0461 (9)	0.0104 (10)	0.0177 (9)	-0.0061 (8)
S1	0.0912 (6)	0.0968 (6)	0.0836 (5)	0.0514 (5)	0.0231 (4)	0.0125 (4)

Table 5. Torsion angles

	Torsion Angle		
C7—C2—C3—C4	-0.3 (4)	C18—C19—C24—C23	-179.7 (2)
C1—C2—C3—C4	-179.3 (3)	C13—C14—C26—C27	110.9 (2)
C2—C3—C4—C5	-0.3 (4)	C15—C14—C26—C27	-16.6 (3)
C3—C4—C5—C6	0.3 (4)	C13—C14—C26—C30	-76.5 (2)
C3—C4—C5—S1	174.3 (2)	C15—C14—C26—C30	156.01 (18)
C4—C5—C6—C7	0.3 (4)	C30—C26—C27—O4	-175.35 (18)
S1—C5—C6—C7	-173.5 (2)	C14—C26—C27—O4	-2.9 (3)
C5—C6—C7—C2	-1.0 (4)	C30—C26—C27—C28	3.9 (3)
C3—C2—C7—C6	1.0 (4)	C14—C26—C27—C28	176.31 (18)
C1—C2—C7—C6	180.0 (3)	O4—C27—C28—C29	179.06 (17)

Table 5. Continued

C13—C8—C9—C10	-0.3 (4)	C26—C27—C28—C29	-0.2 (3)
N1—C8—C9—C10	176.5 (2)	O4—C27—C28—C34	-4.0 (3)
C8—C9—C10—C11	-2.4 (4)	C26—C27—C28—C34	176.8 (2)
C9—C10—C11—C12	2.4 (4)	C34—C28—C29—O5	-178.16 (19)
C10—C11—C12—C13	0.2 (4)	C27—C28—C29—O5	-1.0 (3)
C11—C12—C13—C8	-2.8 (3)	C34—C28—C29—C31	-0.1 (3)
C11—C12—C13—C14	171.8 (2)	C27—C28—C29—C31	177.10 (19)
C9—C8—C13—C12	2.9 (3)	C27—C26—C30—O6	174.4 (2)
N1—C8—C13—C12	-174.0 (2)	C14—C26—C30—O6	1.6 (3)
C9—C8—C13—C14	-172.1 (2)	C27—C26—C30—O5	-6.3 (3)
N1—C8—C13—C14	11.0 (3)	C14—C26—C30—O5	-179.08 (17)
C12—C13—C14—C26	9.4 (3)	O5—C29—C31—C32	177.3 (2)
C8—C13—C14—C26	-175.91 (19)	C28—C29—C31—C32	-0.9 (3)
C12—C13—C14—C15	135.9 (2)	C29—C31—C32—C33	0.9 (4)
C8—C13—C14—C15	-49.4 (2)	C31—C32—C33—C34	0.1 (4)
C26—C14—C15—C17	-74.2 (2)	C32—C33—C34—C28	-1.1 (4)
C13—C14—C15—C17	155.28 (17)	C29—C28—C34—C33	1.0 (3)
C26—C14—C15—C18	45.1 (2)	C27—C28—C34—C33	-175.9 (2)
C13—C14—C15—C18	-85.4 (2)	C9—C8—N1—C16	-135.3 (2)
C26—C14—C15—C16	164.87 (18)	C13—C8—N1—C16	41.6 (3)
C13—C14—C15—C16	34.4 (2)	C9—C8—N1—S1	69.7 (3)
C17—C15—C16—N1	-105.5 (2)	C13—C8—N1—S1	-113.4 (2)
C18—C15—C16—N1	133.9 (2)	C15—C16—N1—C8	-53.5 (3)
C14—C15—C16—N1	13.6 (3)	C15—C16—N1—S1	101.3 (2)
C18—C15—C17—N2	-148 (6)	C23—C24—O3—C25	13.7 (4)
C14—C15—C17—N2	-29 (6)	C19—C24—O3—C25	-166.2 (2)
C16—C15—C17—N2	93 (6)	C26—C27—O4—C18	-9.8 (3)
C17—C15—C18—O4	58.9 (2)	C28—C27—O4—C18	170.96 (16)
C14—C15—C18—O4	-58.6 (2)	C19—C18—O4—C27	165.90 (17)
C16—C15—C18—O4	179.53 (17)	C15—C18—O4—C27	40.9 (2)
C17—C15—C18—C19	-61.1 (2)	C31—C29—O5—C30	-179.81 (19)
C14—C15—C18—C19	-178.57 (18)	C28—C29—O5—C30	-1.6 (3)
C16—C15—C18—C19	59.6 (2)	O6—C30—O5—C29	-175.4 (2)
O4—C18—C19—C20	-47.5 (3)	C26—C30—O5—C29	5.2 (3)
C15—C18—C19—C20	75.3 (3)	C8—N1—S1—O2	-179.7 (2)
O4—C18—C19—C24	130.6 (2)	C16—N1—S1—O2	27.3 (2)
C15—C18—C19—C24	-106.6 (2)	C8—N1—S1—O1	-49.7 (2)
C24—C19—C20—C21	1.3 (4)	C16—N1—S1—O1	157.22 (19)
C18—C19—C20—C21	179.5 (2)	C8—N1—S1—C5	64.5 (2)
C19—C20—C21—C22	-0.7 (4)	C16—N1—S1—C5	-88.5 (2)
C20—C21—C22—C23	0.1 (5)	C6—C5—S1—O2	-17.5 (2)
C21—C22—C23—C24	-0.3 (5)	C4—C5—S1—O2	168.6 (2)
C22—C23—C24—O3	-178.9 (3)	C6—C5—S1—O1	-150.6 (2)
C22—C23—C24—C19	1.0 (4)	C4—C5—S1—O1	35.5 (2)
C20—C19—C24—O3	178.4 (2)	C6—C5—S1—N1	95.9 (2)
C18—C19—C24—O3	0.3 (3)	C4—C5—S1—N1	-78.0 (2)
C20—C19—C24—C23	-1.5 (4)		

N1-S1-C5 [105.85(1)°] angles deviating from ideal tetrahedral values are attributed to the Thrope-Ingold effect[16]. The sum of bond angles around N1 (354.9°) indicates that N1 is in sp^2 hybridization. The Pyridine ring (N1-C8-C13-C14-C15-C16) adopts boat conformation [q2 = 0.621(2) Å, q3 = 0.007(2) Å, φ2 = 89.37(2)°] and pyran ring (O4-C18-C15-C14-C26-C27) adopts a sofa conformation [q2 = 0.380(2) Å, q3 = 0.293(2) Å, φ2 = 127.65(2)°] defined by the above puckering parameters[16]. The dihedral angle between the two mean-planes being 42.54(7)°. The planar atoms of the pyran ring and coumarin ring (C26/C27/C28/C29/O5/C30/C31/C32/C33/C34) are almost co-planar with dihedral angle between the meanplanes being 5.58(4)°. Moreover, methylphenyl ring attached pyridine ring and methoxyphenyl ring attached pyran rings were tilted with the dihedral angle of 39.07(8)° and 69.67(6)° respectively. Crystal structure is stabilized by C-H…O intra molecular hydrogen bond interactions.

4. Conclusions

The title compound is crystallized from ethyl acetate solution by slow evaporation technique. The structure is determined using Direct Methods Protocol and refined using Least-squares Fit methods. The final R factor is 4.10%. As 3D structure is determined now, with the biological importance of such derivatives, the usefulness of the present derivative can be established using Bioinformatics tools.

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