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Crystal and Molecular Structure of 4,6-Dimethyl-9-phenyl-8,12-dioxa-4,6-diazatetracyclo [8.8.0.02,7.013,18]octadeca-2(7),13,15,17-tetraene-3,5,11-trione 2-ethoxyphenyl (2E)-but-2-enoate

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Abstract

The crystal structure of the potential active 4,6-dimethyl-9-phenyl-8,12-dioxa-4,6-diazatetracyclo [8.8.0.02,7.013,18] octadeca-2(7),13,15,17-tetraene-3,5,11-trione 2-ethoxyphenyl (2E)-but-2-enoate ($C_{22}H_{18}N_2O_5$) has been determined from single crystal X-ray diffraction data. In the title compound crystallizes in the monoclinic space group P_12_1/c_1 with unit cell dimension a=15.2039(8), b=12.3888(6) and c= 9.8162(5) [alpha & gamma=90° beta=98.113(2)]. In the structure fused pyrone and pyran rings each adopt a sofa/envelop conformation. The crystal structure is stabilized by intramolecular C-H...O hydrogen bond interaction.

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

1. Introduction

Coumarine derivatives 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, anti-inflammatory and analgesic activities have been published[1]. 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]. Hence we started working on these derivatives having a wide variety of pharmacological activities and here we report the crystal structure of the title compound.

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2. Experimental Section

2.1. Material

With the collaboration of Organic Chemistry Department at University of Madras, we obtained the title compound and it is crystallized.

2.2. Methods

Diffraction quality crystals were obtained by slow evaporation of a solution in ethyl acetate and the obtained crystals were analyzed using single crystal X-ray diffractometer.

2.3. Synthesis of the Title Compound

A mixture of 2-formylphenyl (2E)-3-phenylprop-2-enoate (0.252 g, 1 mmol) and N, N-dimethylbarbituric acid (0.156 g, 1 mmol) was placed in a round bottom flask and melted at 180°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 prod-

uct in 97% yield as colorless solid. 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.

2.4. X-Ray Crystallography

For the crystal structure determination, the single crystal of the compound $C_{22}H_{18}N_2O_5$ 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: 931519. 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 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 angles; Table 4 shows anisotropic displacement parameters, Table 5 shows the hydrogen coordinates and Table 6 shows the torsion angles. Table 7 shows hydrogen-bond geometry (See Supporting Information).

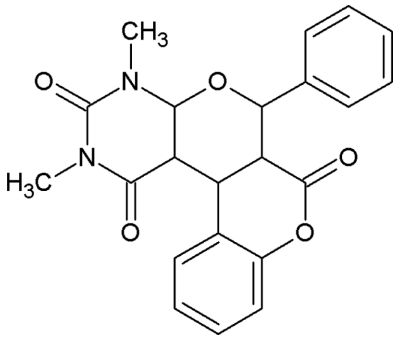

Fig. 1. Schematic diagram of the molecule

Table 1. Crystal data and structure refinement

Empirical formula	$C_{22}H_{18}N_2O_5$
Formula weight	390.38
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 15.204 (8)Å
	b = 12.389 (6)Å β = 98.113(2)°
	c = 9.816 (5)Å
Volume	1830.46 (16)Å^3
Z, Calculated density	4, 1.417 Mg/m^3
Absorption coefficient	0.102 mm^{-1}
F(000)	816
Crystal size	0.30 × 0.30 × 0.25 mm
θ range for data collection	2.05 to 28.21°
Limiting indices	-17<=h<=17, -14<=k<=12, -11<=l<=11
Reflections collected / unique	14679/2932 [Rint = 0.0319]
Completeness to θ = 25.00	Completeness to θ = 24.19, 99.5%
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	2932 / 0 / 264
Goodness-of-fit on F2	1.06
Final R indices [I>2σ(I)]	R1 = 0.0457, wR2 = 0.1264
R indices (all data)	R1 = 0.0675, wR2 = 0.1530
Largest diff. peak and hole	-0.176 and 0.313 e.Å^{-3}

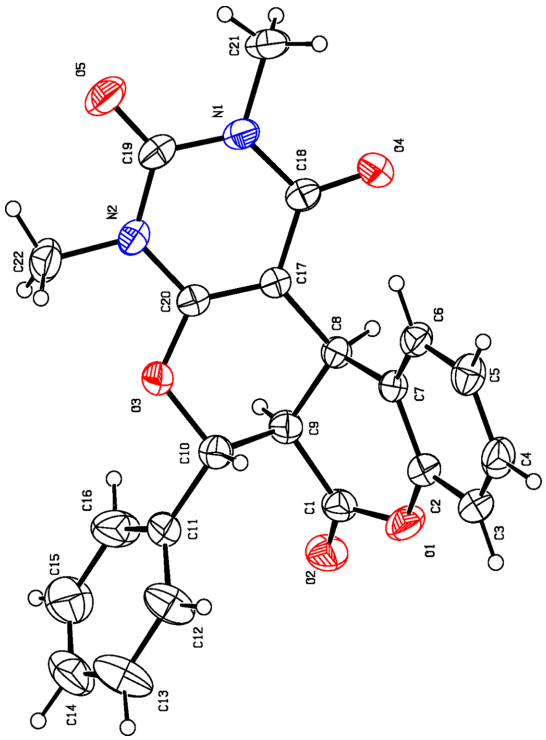

Fig. 2. Displacement ellipsoids are drawn at the 30% probability level.

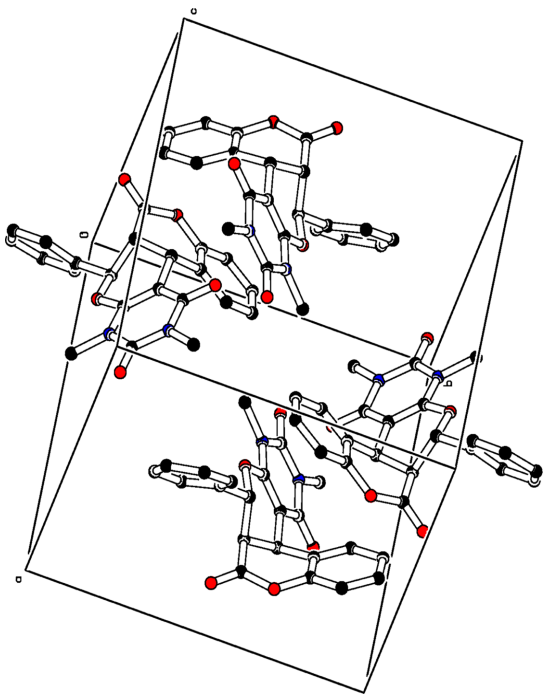

Fig. 3. Crystal packing of the title compound, H atoms have been omitted for clarity.

3. Results and Discussion

Title compound crystallizes in the monoclinic centrosymmetric space group P121/c1 with Z = 4. The structure of the compound consists of coumarine, pyran, and diazacyclic fragments whose rings are connected to one another. All the three rings exhibit coplanarity with one another. Similar kind of ring systems has been observed in our previous study and its bond length, bond angle, and torsion angles are almost similar to the title compound. The structure report has been described in jagadeesan[15(a,b)].

In the molecule, the pyrone (O1-C2-C7-C8-C9-C1) and pyran (O3-C20-C17-C8-C9-C10) rings adopt C9-envelope or sofa conformations with C9 atom displaced by the bond length 0.603 (2) **Å** and 0.668 (2) **Å**, respectively, and defined by the least-square planes formed by the remaining ring atoms. This can also be confirmed by the asymmetry parameters described by Nardelli *et al.* in 1983[16] {six-membered pyrone ring of the coumarine ring system [DS (C9) =0.129(2) **Å** and D2 (C9-C8) =0.008(1) **Å**] and pyran ring [DS (C10) =0.186(1) **Å** and D2 (C10-C9) =0.033(1) **Å**]}; Pyran ring and phenyl rings are tilted to one another by forming the dihedral angle 74.51(1)°. The torsion angles defined by the atoms H8-C8-C9-H9 (-49.7°) and H9-C9-C10-H10 (-170.2°), describes the ring fusion in six membered pyrone ring of the coumarine moiety and pyran ring system respectively. The pyrone and pyran rings which lie on two mean-planes makes the dihedral angle of 56.80 (6)°. The pyran ring and diazacyclic ring (N1-N2-C17-C18-C19-C20) orients in such a way that they are almost co-planar with one another defined by the dihedral angle 7.41(7)°. Moreover, the planar atoms of the pyrone ring and benzene ring (C2-C3-C4-C5-C6-C7) of the coumarine moiety are also co-planar which is also been defined by the dihedral angle of 13.11 (7)°. No Classic intermolecular hydrogen bonds has been observed in the crystal packing and further the crystal structure is stabilized by intramolecular C21-H21(c)…O5 and C22-H22(a)...O5 hydrogen bond interactions (Fig. 3 shows crystal packing diagram of molecule).

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

Atom	X	y	z	U_{iso}*/U_{eq}
C1	0.12190 (16)	0.0779 (2)	0.3703 (3)	0.0524 (6)
C2	0.13454 (16)	0.2647 (2)	0.3121 (3)	0.0505 (6)
C3	0.08848 (18)	0.3485 (2)	0.2449 (3)	0.0607 (7)
C4	0.13332 (18)	0.4402 (2)	0.2169 (3)	0.0614 (7)
C5	0.22358 (18)	0.4467 (2)	0.2560 (3)	0.0577 (7)
C6	0.26866 (16)	0.36123 (19)	0.3239 (3)	0.0491 (6)
C7	0.22545 (14)	0.26855 (18)	0.3539 (2)	0.0410 (5)
C8	0.27013 (14)	0.17156 (18)	0.4279 (2)	0.0414 (5)
C9	0.22138 (15)	0.06865 (19)	0.3763 (3)	0.0482 (6)
C10	0.24454 (15)	0.0414 (2)	0.2341 (3)	0.0507 (6)
C11	0.19638 (16)	-0.0543 (2)	0.1651 (3)	0.0532 (7)
C12	0.1358 (2)	-0.0393 (3)	0.0516 (3)	0.0823 (10)
C13	0.0897 (3)	-0.1270 (4)	-0.0102 (4)	0.1081 (14)
C14	0.1048 (3)	-0.2285 (3)	0.0395 (4)	0.0956 (12)
C15	0.1621 (3)	-0.2429 (3)	0.1555 (6)	0.1169 (15)
C16	0.2073 (2)	-0.1555 (3)	0.2182 (5)	0.1045 (14)
C17	0.36681 (14)	0.15738 (17)	0.4137 (2)	0.0397 (5)
C18	0.43286 (15)	0.2196 (2)	0.4966 (3)	0.0479 (6)
C19	0.54781 (16)	0.1186 (2)	0.3978 (3)	0.0541 (7)
C20	0.39280 (14)	0.08053 (18)	0.3320 (2)	0.0417 (5)
C21	0.59128 (18)	0.2662 (3)	0.5544 (3)	0.0751 (9)
C22	0.50574 (18)	-0.0241 (2)	0.2303 (3)	0.0698 (8)
N1	0.52142 (12)	0.19906 (17)	0.4785 (2)	0.0522 (5)
N2	0.48082 (12)	0.05777 (15)	0.3254 (2)	0.0489 (5)
O1	0.08397 (11)	0.17489 (15)	0.3381 (2)	0.0657 (6)
O2	0.07520 (11)	0.00462 (16)	0.3917 (2)	0.0684 (6)
O3	0.33943 (10)	0.01440 (13)	0.25085 (17)	0.0505 (5)
O4	0.41783 (12)	0.28941 (16)	0.57856 (19)	0.0664 (5)
O5	0.62571 (11)	0.10055 (17)	0.3908 (2)	0.0776 (6)

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

Atom	Bond Angle (º)	Atom	Bond Angle (º)
C1—O2	1.190 (3)	C12—H12	0.9300
C1—O1	1.351 (3)	C13—C14	1.356 (5)
C1—C9	1.510 (3)	C13—H13	0.9300
C2—C3	1.368 (4)	C14—C15	1.345 (6)
C2—C7	1.386 (3)	C14—H14	0.9300
C2—O1	1.396 (3)	C15—C16	1.380 (5)
C3—C4	1.373 (4)	C15—H15	0.9300
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.374 (4)	C17—C20	1.340 (3)
C4—H4	0.9300	C17—C18	1.427 (3)
C5—C6	1.381 (3)	C18—O4	1.224 (3)
C5—H5	0.9300	C18—N1	1.406 (3)
C6—C7	1.375 (3)	C19—O5	1.217 (3)
C6—H6	0.9300	C19—N1	1.368 (3)
C7—C8	1.514 (3)	C19—N2	1.380 (3)
C8—C17	1.506 (3)	C20—O3	1.335 (3)
C8—C9	1.525 (3)	C20—N2	1.378 (3)
C8—H8	0.9800	C21—N1	1.467 (3)
C9—C10	1.525 (4)	C21—H21A	0.9600
C9—H9	0.9800	C21—H21B	0.9600

Table 3. Continued

Atom	Bond Angle (º)	Atom	Bond Angle (º)
C10—O3	1.467 (3)	C21—H21C	0.9600
C10—C11	1.503 (3)	C22—N2	1.464 (3)
C10—H10	0.9800	C22—H22A	0.9600
C11—C12	1.355 (4)	C22—H22B	0.9600
C11—C16	1.359 (4)	C22—H22C	0.9600
C12—C13	1.386 (4)		
O2—C1—O1	118.3 (2)	C14—C13—C12	121.3 (3)
O2—C1—C9	123.7 (2)	C14—C13—H13	119.3
O1—C1—C9	118.0 (2)	C12—C13—H13	119.3
C3—C2—C7	122.5 (2)	C15—C14—C13	119.0 (3)
C3—C2—O1	115.8 (2)	C15—C14—H14	120.5
C7—C2—O1	121.7 (2)	C13—C14—H14	120.5
C2—C3—C4	119.3 (2)	C14—C15—C16	119.7 (4)
C2—C3—H3	120.3	C14—C15—H15	120.1
C4—C3—H3	120.3	C16—C15—H15	120.1
C3—C4—C5	119.8 (2)	C11—C16—C15	121.8 (4)
C3—C4—H4	120.1	C11—C16—H16	119.1
C5—C4—H4	120.1	C15—C16—H16	119.1
C4—C5—C6	119.9 (2)	C20—C17—C18	118.8 (2)
C4—C5—H5	120.1	C20—C17—C8	120.8 (2)
C6—C5—H5	120.1	C18—C17—C8	120.1 (2)
C7—C6—C5	121.6 (2)	O4—C18—N1	118.8 (2)
C7—C6—H6	119.2	O4—C18—C17	125.1 (2)
C5—C6—H6	119.2	N1—C18—C17	116.1 (2)
C6—C7—C2	116.9 (2)	O5—C19—N1	122.3 (2)
C6—C7—C8	124.7 (2)	O5—C19—N2	121.6 (3)
C2—C7—C8	118.4 (2)	N1—C19—N2	116.1 (2)
C17—C8—C7	115.19 (18)	O3—C20—C17	126.0 (2)
C17—C8—C9	107.86 (18)	O3—C20—N2	111.05 (19)
C7—C8—C9	109.87 (18)	C17—C20—N2	122.9 (2)
C17—C8—H8	107.9	N1—C21—H21A	109.5
C7—C8—H8	107.9	N1—C21—H21B	109.5
C9—C8—H8	107.9	H21A—C21—H21B	109.5
C1—C9—C10	109.9 (2)	N1—C21—H21C	109.5
C1—C9—C8	112.73 (19)	H21A—C21—H21C	109.5
C10—C9—C8	108.98 (19)	H21B—C21—H21C	109.5
C1—C9—H9	108.4	N2—C22—H22A	109.5
C10—C9—H9	108.4	N2—C22—H22B	109.5
C8—C9—H9	108.4	H22A—C22—H22B	109.5
O3—C10—C11	106.24 (19)	N2—C22—H22C	109.5
O3—C10—C9	107.35 (19)	H22A—C22—H22C	109.5
C11—C10—C9	115.2 (2)	H22B—C22—H22C	109.5
O3—C10—H10	109.3	C19—N1—C18	124.7 (2)
C11—C10—H10	109.3	C19—N1—C21	117.2 (2)
C9—C10—H10	109.3	C18—N1—C21	118.1 (2)
C12—C11—C16	118.3 (3)	C20—N2—C19	121.0 (2)
C12—C11—C10	119.6 (2)	C20—N2—C22	120.8 (2)
C16—C11—C10	122.0 (3)	C19—N2—C22	117.9 (2)
C11—C12—C13	119.7 (3)	C1—O1—C2	121.57 (18)
C11—C12—H12	120.1	C20—O3—C10	115.62 (17)
C13—C12—H12	120.1		

Table 4. Anisotropic displacement parameters (Å^2)

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0441 (13)	0.0582 (16)	0.0556 (15)	-0.0107 (13)	0.0097 (11)	-0.0096 (13)
C2	0.0414 (13)	0.0523 (14)	0.0572 (15)	0.0004 (11)	0.0052 (11)	-0.0050 (12)
C3	0.0465 (14)	0.0647 (17)	0.0672 (17)	0.0102 (13)	-0.0053 (13)	-0.0073 (14)
C4	0.0653 (18)	0.0590 (17)	0.0587 (17)	0.0204 (14)	0.0044 (14)	0.0027 (13)
C5	0.0605 (16)	0.0494 (15)	0.0660 (17)	0.0054 (12)	0.0181 (13)	0.0070 (13)
C6	0.0406 (12)	0.0494 (14)	0.0587 (15)	0.0016 (11)	0.0113 (11)	-0.0008 (12)
C7	0.0376 (12)	0.0463 (13)	0.0403 (12)	0.0009 (10)	0.0093 (10)	-0.0062 (10)
C8	0.0389 (12)	0.0454 (13)	0.0408 (13)	-0.0018 (10)	0.0086 (10)	-0.0030 (10)
C9	0.0455 (13)	0.0466 (13)	0.0528 (14)	-0.0047 (11)	0.0084 (11)	-0.0023 (11)
C10	0.0478 (14)	0.0489 (14)	0.0543 (15)	-0.0010 (11)	0.0034 (11)	-0.0015 (11)
C11	0.0501 (14)	0.0492 (15)	0.0600 (16)	-0.0035 (11)	0.0073 (12)	-0.0079 (12)
C12	0.109 (3)	0.079 (2)	0.0531 (18)	-0.0248 (19)	-0.0093 (17)	0.0007 (16)
C13	0.135 (3)	0.116 (3)	0.063 (2)	-0.046 (3)	-0.019 (2)	-0.012 (2)
C14	0.105 (3)	0.081 (3)	0.102 (3)	-0.036 (2)	0.020 (2)	-0.035 (2)
C15	0.108 (3)	0.054 (2)	0.178 (5)	0.000 (2)	-0.018 (3)	-0.013 (3)
C16	0.086 (2)	0.057 (2)	0.152 (4)	0.0067 (17)	-0.049 (2)	-0.007 (2)
C17	0.0372 (11)	0.0407 (12)	0.0407 (12)	-0.0004 (10)	0.0042 (10)	0.0017 (10)
C18	0.0423 (13)	0.0533 (15)	0.0467 (14)	0.0022 (11)	0.0016 (11)	0.0054 (12)
C19	0.0394 (14)	0.0584 (15)	0.0638 (16)	0.0057 (12)	0.0045 (12)	0.0117 (13)
C20	0.0392 (12)	0.0424 (12)	0.0430 (12)	-0.0010 (10)	0.0042 (10)	0.0061 (11)
C21	0.0442 (15)	0.083 (2)	0.091 (2)	-0.0071 (14)	-0.0149 (15)	-0.0078 (17)
C22	0.0601 (16)	0.0663 (18)	0.089 (2)	0.0089 (14)	0.0296 (15)	-0.0104 (16)
N1	0.0371 (11)	0.0597 (13)	0.0573 (13)	0.0003 (9)	-0.0018 (9)	-0.0001 (11)
N2	0.0410 (11)	0.0490 (12)	0.0579 (13)	0.0064 (9)	0.0109 (9)	0.0022 (10)
O1	0.0359 (9)	0.0604 (12)	0.1003 (15)	-0.0031 (8)	0.0072 (9)	0.0003 (10)
O2	0.0540 (11)	0.0708 (12)	0.0825 (14)	-0.0237 (10)	0.0164 (10)	-0.0083 (10)
O3	0.0435 (9)	0.0512 (10)	0.0577 (10)	-0.0023 (8)	0.0102 (8)	-0.0117 (8)
O4	0.0565 (11)	0.0762 (13)	0.0645 (12)	-0.0037 (9)	0.0020 (9)	-0.0257 (11)
O5	0.0398 (11)	0.0849 (14)	0.1081 (16)	0.0078 (10)	0.0108 (10)	-0.0005 (12)

Table 5. Hydrogen coordinates (Å^2)

Atom	x	y	z	Uiso*/Ueq
H22A	0.5693	-0.0300	0.2406	0.105*
H22B	0.4835	-0.0035	0.1376	0.105*
H22C	0.4807	-0.0924	0.2506	0.105*
H12	0.1252	0.0296	0.0153	0.099*
H10	0.2336	0.1047	0.1742	0.061*
H9	0.2423	0.0097	0.4392	0.058*
H8	0.2656	0.1790	0.5260	0.050*
H6	0.3297	0.3665	0.3500	0.059*
H5	0.2542	0.5086	0.2368	0.069*
H4	0.1027	0.4977	0.1715	0.074*
H3	0.0274	0.3433	0.2185	0.073*
H13	0.0475	-0.1160	-0.0873	0.130*
H14	0.0760	-0.2872	-0.0060	0.115*
H15	0.1712	-0.3115	0.1934	0.140*
H16	0.2463	-0.1662	0.2989	0.125*
H21A	0.6028	0.2422	0.6483	0.113*
H21B	0.5722	0.3401	0.5518	0.113*
H21C	0.6446	0.2601	0.5128	0.113*

Table 6. Torsion angles [°]

C7—C2—C3—C4	0.2 (4)	C14—C15—C16—C11	-0.7 (7)
O1—C2—C3—C4	179.3 (2)	C7—C8—C17—C20	-105.6 (2)
C2—C3—C4—C5	0.2 (4)	C9—C8—C17—C20	17.5 (3)
C3—C4—C5—C6	-0.3 (4)	C7—C8—C17—C18	79.9 (3)
C4—C5—C6—C7	0.0 (4)	C9—C8—C17—C18	-157.0 (2)
C5—C6—C7—C2	0.3 (3)	C20—C17—C18—O4	-177.4 (2)
C5—C6—C7—C8	-180.0 (2)	C8—C17—C18—O4	-2.8 (4)
C3—C2—C7—C6	-0.5 (4)	C20—C17—C18—N1	3.9 (3)
O1—C2—C7—C6	-179.5 (2)	C8—C17—C18—N1	178.55 (19)
C3—C2—C7—C8	179.9 (2)	C18—C17—C20—O3	178.6 (2)
O1—C2—C7—C8	0.8 (3)	C8—C17—C20—O3	4.0 (3)
C6—C7—C8—C17	-26.3 (3)	C18—C17—C20—N2	0.8 (3)
C2—C7—C8—C17	153.4 (2)	C8—C17—C20—N2	-173.7 (2)
C6—C7—C8—C9	-148.3 (2)	O5—C19—N1—C18	-176.2 (2)
C2—C7—C8—C9	31.3 (3)	N2—C19—N1—C18	3.1 (4)
O2—C1—C9—C10	91.7 (3)	O5—C19—N1—C21	1.8 (4)
O1—C1—C9—C10	-87.9 (3)	N2—C19—N1—C21	-178.9 (2)
O2—C1—C9—C8	-146.5 (2)	O4—C18—N1—C19	175.2 (2)
O1—C1—C9—C8	33.9 (3)	C17—C18—N1—C19	-6.1 (3)
C17—C8—C9—C1	-173.48 (19)	O4—C18—N1—C21	-2.8 (3)
C7—C8—C9—C1	-47.2 (3)	C17—C18—N1—C21	175.9 (2)
C17—C8—C9—C10	-51.1 (2)	O3—C20—N2—C19	177.9 (2)
C7—C8—C9—C10	75.2 (2)	C17—C20—N2—C19	-4.1 (3)
C1—C9—C10—O3	-170.04 (19)	O3—C20—N2—C22	4.4 (3)
C8—C9—C10—O3	65.9 (2)	C17—C20—N2—C22	-177.5 (2)
C1—C9—C10—C11	-51.9 (3)	O5—C19—N2—C20	-178.6 (2)
C8—C9—C10—C11	-175.94 (19)	N1—C19—N2—C20	2.1 (3)
O3—C10—C11—C12	-129.3 (3)	O5—C19—N2—C22	-5.0 (4)
C9—C10—C11—C12	112.0 (3)	N1—C19—N2—C22	175.7 (2)
O3—C10—C11—C16	55.1 (4)	O2—C1—O1—C2	179.8 (2)
C9—C10—C11—C16	-63.6 (4)	C9—C1—O1—C2	-0.6 (3)
C16—C11—C12—C13	-2.6 (5)	C3—C2—O1—C1	162.7 (2)
C10—C11—C12—C13	-178.4 (3)	C7—C2—O1—C1	-18.2 (4)
C11—C12—C13—C14	-1.0 (6)	C17—C20—O3—C10	10.6 (3)
C12—C13—C14—C15	3.8 (7)	N2—C20—O3—C10	-171.39 (18)
C13—C14—C15—C16	-3.0 (7)	C11—C10—O3—C20	-168.50 (19)
C12—C11—C16—C15	3.5 (6)	C9—C10—O3—C20	-44.7 (3)
C10—C11—C16—C15	179.1 (4)		

Table 7. Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H(Å)	H···*A*(Å)	*D*···*A*(Å)	*D*—H···*A*(°)
C21-H21*C*···O5	0.96	2.30	2.702 (4)	104
C22—22*A*···O5	0.96	2.27	2.717 (4)	107

4. Conclusions

Crystal structure of a novel coumarine based derivatives having a wide range of applications is described. The title compound is insoluble in millipore water and it is crystallized in ethyl acetate by slow evaporation techinique. The pyrone and pyran rings adopt a sofa or envelop conformation. In general the coumarine deriv-

atives are well characterized interms of medicinal and biological applications. The title structure may be important from a medicinal point of view as well as their widespread biological significance. The structure may be useful for further investigation on the mechanism, potential activity, optimal reaction condition etc which will be further characterized as a future prospective of our project.

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