

Crystal Structure Theory and Applications of 14-Ethoxy-4,6,-dimethyl-8.12-dioxa-4.6-diazatetracyclo [8.8.0.0^{2,7}.0^{13,18}]octadeca-13,15,17-triene-3,5-dione

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Abstract

In view of the growing medicinal importance of chromene and its derivatives, the single crystal X-ray diffraction study was carried out for the potential active 4,6-dimethyl-9-phenyl-8,12-dioxa-4,6-diazatetracyclo [8.8.0.0^{2,7}.0^{13,18}]octadeca-2(7),13,15,17-tetraene-3,5,11-trione-2-ethoxyphenyl (2E)-but-2-enoate (C₁₈H₂₀N₂O₅). In the title compound are two molecules exist in the asymmetric unit. It crystallizes in the monoclinic space group P2₁/c with unit cell dimension a=14.608(3) Å, b=12.845(3) and c= 17.781(4) [alpha & gamma=90° beta=91.233(5)°]. Both pyran and pyran ring of the chromene moiety adopts sofa conformation in the molecule A & B. The crystal structure is stabilized by intramolecular C-H...O hydrogen bond interaction.

Keywords: Pyran; Chromene; Sofa Conformation; Single Crystal Structure; X-ray Diffraction (XRD)

1. Introduction

The chromene moiety regularly appears as a principal structural component in various biologically important organic compounds such as flavonoids, natural alkaloids, tocopherols and anthocyanins^[1]. It is an essential synthon for the synthesis of a variety of natural products, including hematoxylin, clausenin, brazilin and ripariochromene^[2] chromenes constitute one of the main class of naturally occurring oxygen heterocycles, which posses several biological and pharmacological properties such as anti-coagulant, anti-sterility, antiviral, anti-fungal, anti-inflammatory, cardionthonic, anti-diabetic, spasmolytic, diuretic, anti-anaphylactic, anti-cancer activities^[3-12] and also useful in treatment of Schizophrenia and Alzheimer's diseases^[13,14]. Recently, the structural modification of chromene scaffold with the addition of heterocyclic substituent's at either the second or third position has attracted extensive interest in the field of structure based drug designing (SBDD).

In view of the growing medicinal importance of chromene and its derivatives, the single crystal X-ray diffraction study was carried out for one such compound.

2. 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 round 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 5.0%.

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3. Experimental

3.1. Synthesis of the Title Compound

A mixture of 2-(allyloxy)-3-ethoxybenzaldehyde (0.206 g, 1 mmol) and *N,N*-dimethylbarbutric acid (0.156 g, 1 mmol) was placed in a round bottom flask and melted at 180°C for 1h. 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 a colorless solid. Good crystals of this compound suitable for X-ray diffraction studies were obtained by recrystallization from the solution of ethylacetate.

3.2. 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^[15]. The MoK α radiation of wavelength, (λ =

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 $F_2 > 2\sigma(F_2)$. The structures were solved by direct methods using SHELXS-97 and refined by a full-matrix least-squares procedure using the program SHELXL-97^[16,17]. 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^[18] and PLATON^[19]. The software used to prepare material for publication is WinGX publication routines^[20]. Experimental data are listed in Table 1. CCDC reference number: 930756. 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

Table 1. Crystal data and structure refinement

Empirical formula	$C_{18}H_{20}N_2O_5$
Formula weight	344.36
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
space group	$P2_1/c$
Unit cell dimensions	$a = 14.608 (3) \text{ \AA}$ $b = 12.845 (3) \text{ \AA}$ $c = 17.781 (4) \text{ \AA}$ $\beta = 91.233 (5)^\circ$
Volume	$3335.7 (12) \text{ \AA}^3$
Z, Calculated density	8, 1.371 Mg/m ³
Absorption coefficient	0.10 mm ⁻¹
F(000)	1456
Crystal size (mm)	0.25×0.35×0.30
θ range for data collection	1.4 to 28.3°
Limiting indices	$-19 \leq h \leq 19$ $-16 \leq k \leq 16$ $-23 \leq l \leq 22$
Reflections collected / unique	32484 / 8214 [$R_{int} = 0.039$]
Completeness to theta	100%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8214 / 0 / 493
Goodness-of-fit on F^2	1.022
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.055$ $wR2 = 0.149$
R indices (all data)	$R1 = 0.103$ $wR2 = 0.170$
Largest diff. peak and hole	0.261 and -0.230 e.Å ⁻³

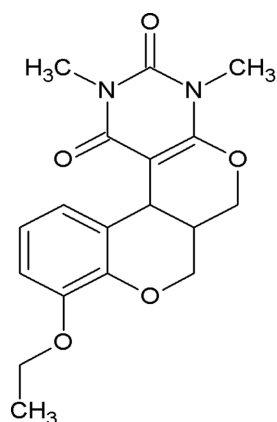


Fig. 1. Schematic diagram of the molecule.

2a and 2b gives the atomic coordinates of the molecule A & molecule B, Fig. 4a and 4b describes the bond lengths of molecule (A and B) and Fig. 5a and 5b describes bond angles of the compound; Table 3a and 3b shows anisotropic displacement parameters for molecule (A and B), Table 4 (a and b) shows the hydrogen coordinates for molecule (A and B) and Table 5a and 5b shows the torsion angles for molecule (A and B) of the compound.

4. Results and Discussion

In the molecular structure of the title compound has two molecules present in the asymmetric unit. In each

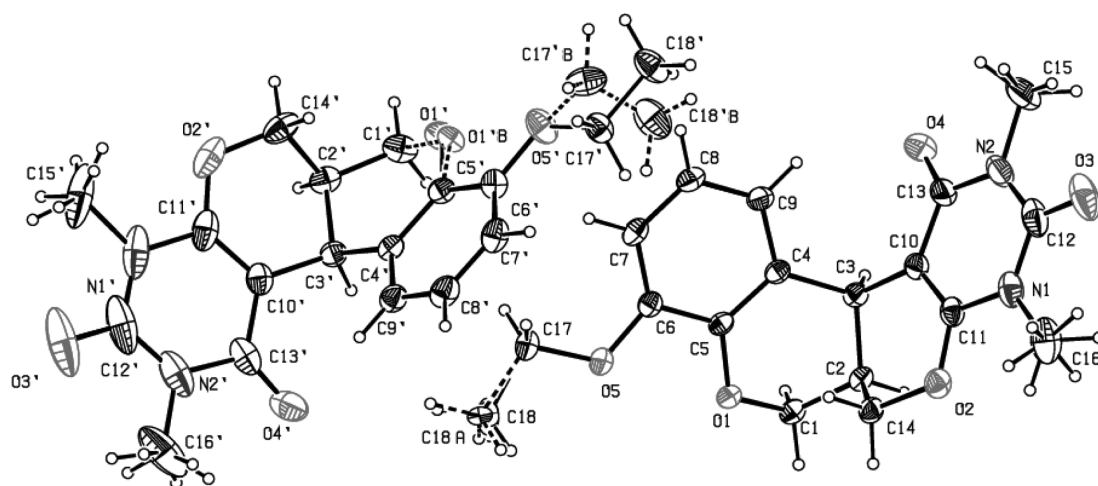


Fig. 2. Displacement ellipsoids are drawn at the 30% probability level.

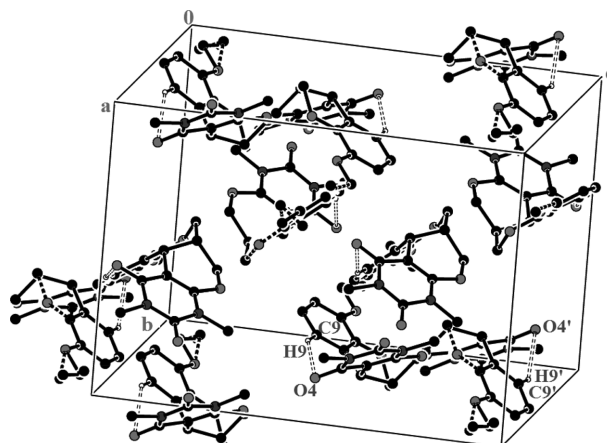


Fig. 3. Crystal packing of the title compound, H atoms have been omitted for clarity.

Table 2a. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the non-hydrogen atoms of molecule A of the compound

Atom	x	y	z	*U(eq)
C1	5051(1)	5143(2)	1339(1)	49(1)
C2	5999(1)	5506(1)	1567(1)	46(1)
C3	6545(1)	5810(2)	878(1)	47(1)
C4	5932(1)	6410(1)	316(1)	45(1)
C5	4992(1)	6463(1)	417(1)	44(1)
C6	4428(1)	7066(2)	-68(1)	48(1)
C7	4806(2)	7576(2)	-672(1)	55(1)
C8	5736(2)	7478(2)	-794(1)	58(1)
C9	6290(1)	6910(2)	-312(1)	53(1)
C10	7393(1)	6405(2)	1142(1)	54(1)
C11	7458(1)	6814(2)	1843(1)	56(1)
C12	8991(2)	7441(2)	1691(2)	90(1)
C13	8190(2)	6440(2)	686(2)	74(1)
C14	5921(1)	6427(2)	2093(1)	52(1)
C15	9731(2)	7169(3)	499(2)	134(2)
C16	8257(2)	7763(2)	2880(2)	106(1)
C17	2903(2)	7624(2)	-373(1)	66(1)
C18	1996(8)	7493(1)	-37(6)	90(3)
C18'A	1923(1)	7589(2)	-75(9)	48(4)
N1	8235(1)	7303(2)	2126(1)	73(1)
N2	8941(1)	7016(2)	982(2)	89(1)
O1	4542(1)	5976(1)	987(1)	51(1)
O2	6807(1)	6789(1)	2359(1)	62(1)
O3	9665(1)	7915(2)	1927(2)	123(1)
O4	8253(1)	6022(2)	71(1)	100(1)
O5	3525(1)	7075(1)	115(1)	59(1)

$$*U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

molecule the pyran ring (C2/C3/C10/C11/O2/C14) in molecule A and (C2'/C3'/C10'/C11'/O2'/C14') in molecule B attached at the C2, C3 and C2', C3' position of chromene moiety [C1-C9/O1 (molecule A) and C1'-C9'/O1' (molecule B)] respectively. Also the diazacyclic ring (C10/C11/N1/C12/N2/C13) in molecule A and (C10'/C11'/N1'/C12'/N2'/C13') in molecule B attached at the C10, C11 and C10', C11' position of the pyran ring.

The ethoxy group attached at the coumarin ring was found to be disordered in both molecules with two positions i.e. C18/C18A in molecule A and C17'/C17B/C18'/C18B in molecule B. The site occupancy factors (SOF) of these two possible sites are converged to be

Table 2b. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the non-hydrogen atoms of molecule B of the compound.

Atom	x	y	z	*U(eq)
C1'	3006(2)	8159(2)	-2738(1)	70(1)
C2'	2034(2)	8516(2)	-2867(1)	62(1)
C3'	1611(1)	8809(2)	-2121(1)	53(1)
C4'	2272(1)	9503(2)	-1666(1)	50(1)
C5'	3194(1)	9519(2)	-1831(1)	52(1)
C6'	3805(2)	10169(2)	-1421(1)	59(1)
C7'	3479(2)	10782(2)	-847(1)	69(1)
C8'	2569(2)	10764(2)	-686(1)	71(1)
C9'	1970(2)	10139(2)	-1084(1)	62(1)
C10'	701(2)	9315(2)	-2264(1)	64(1)
C11'	504(2)	9772(2)	-2925(2)	82(1)
C12'	-988(3)	10327(3)	-2526(4)	139(2)
C13'	12(2)	9264(2)	-1703(2)	84(1)
C14'	1985(2)	9438(2)	-3394(1)	84(1)
C15'	-495(2)	10823(3)	-3786(2)	169(2)
C16'	-1474(2)	9896(3)	-1273(2)	180(2)
C17'	5299(3)	10729(3)	-1121(4)	65(2)
C17'B	5497(1)	10896(9)	-1569(1)	89(4)
C18'	6259(4)	10527(4)	-1365(4)	86(2)
C18'B	5894(1)	10416(1)	-929(1)	111(5)
N1'	-337(2)	10249(2)	-3073(2)	116(1)
N2'	-796(2)	9810(2)	-1873(2)	113(1)
O1'	3625(2)	8931(1)	-2339(2)	47(3)
O1'B	3554(9)	8947(8)	-2414(9)	77(3)
O2'	1059(2)	9820(2)	-3515(1)	101(1)
O3'	-1695(2)	10815(2)	-2648(2)	190(2)

$$*U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

0.292(5)/0.707(5) respectively.

In molecule A, the pyran ring (C1-C5/O1) and phenyl ring (C4-C9) of the chromene moiety are co-planar with dihedral angles of $5.95(6)^\circ$. Pyran oxygen in molecule B was found to be disordered (O1'/O1'') over two sets of sites [site occupancies = 0.292(5) and 0.707(5)]. The terminal hydrogen atoms of methyl group present in the diazacyclic ring at the molecule (A and B) was found to be disordered, with the site occupancy factors (SOF) for each atoms to be 0.5(5), respectively. The AFIX 127 command in SHELXL (Sheldrick, 2008) were used to model the disorder.

Both pyran and pyran ring of the chromene moiety adopts sofa conformation in the molecule A. The puck-

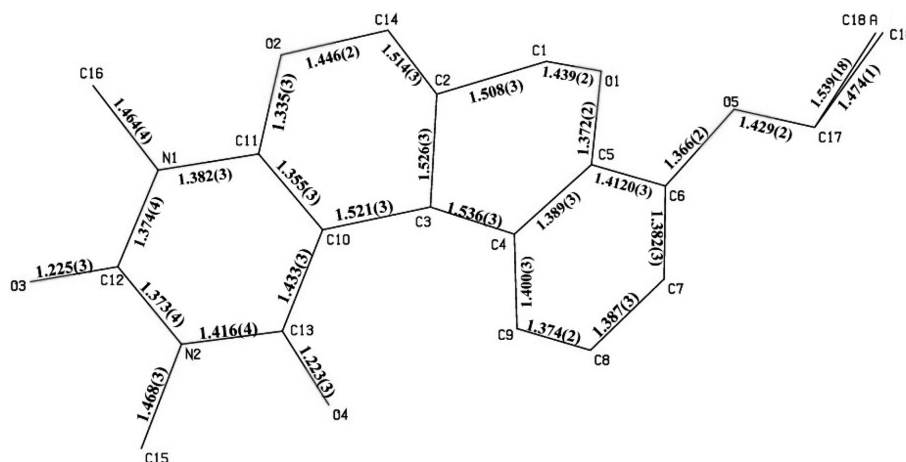


Fig. 4a. Bond length for molecule A of the compound.

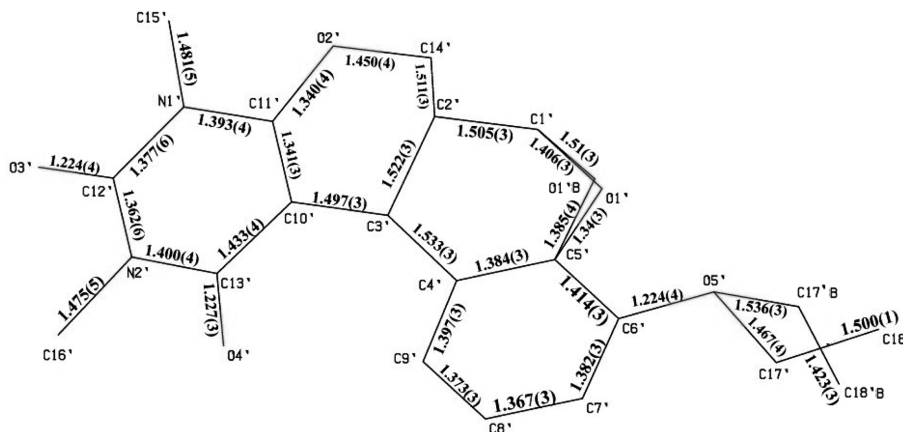


Fig. 4b. Bond length for molecule B of the compound.

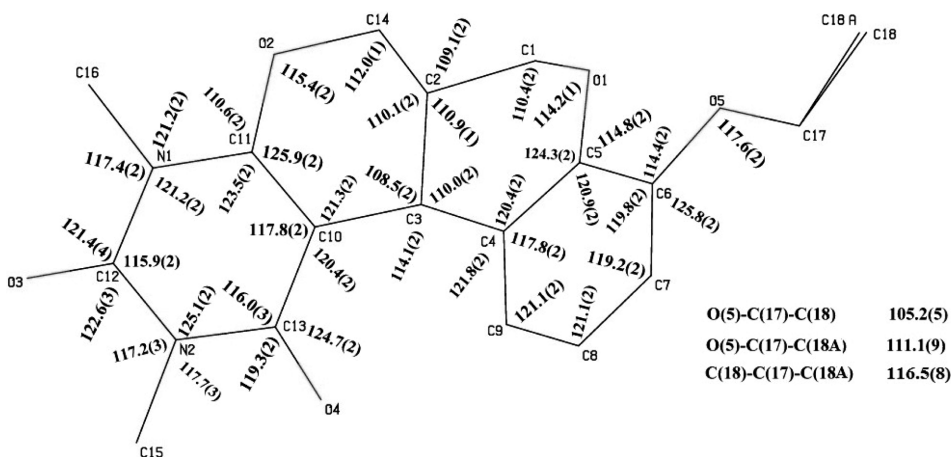


Fig. 5a. Bond Angle for molecule A of the compound.

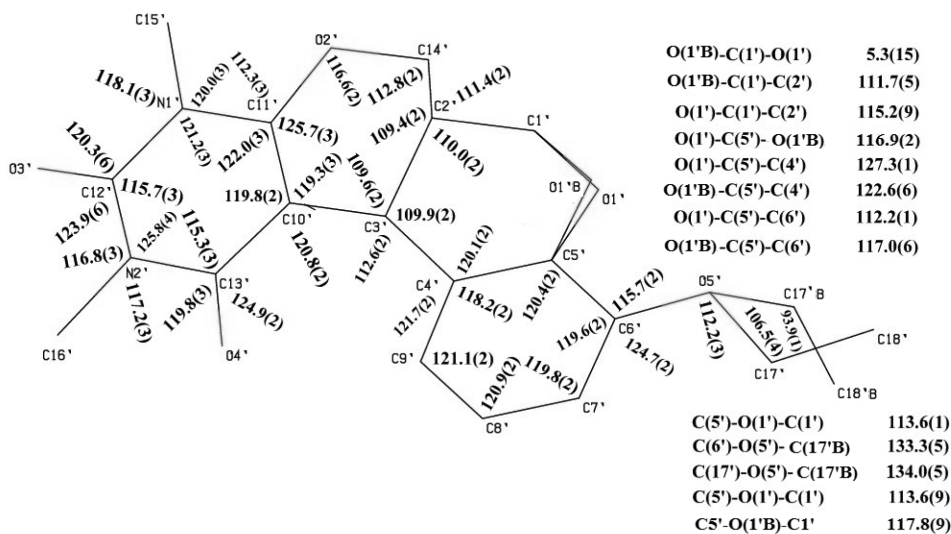


Fig. 5b. Bond Angle for molecule B of the compound.

Table 3a. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the non-hydrogen atoms of molecule A of the compound.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	60(1)	44(1)	44(1)	3(1)	0(1)	-1(1)
C2	55(1)	43(1)	39(1)	2(1)	-2(1)	2(1)
C3	53(1)	45(1)	44(1)	-2(1)	3(1)	6(1)
C4	55(1)	42(1)	37(1)	-4(1)	1(1)	0(1)
C5	55(1)	42(1)	34(1)	-3(1)	1(1)	-1(1)
C6	54(1)	44(1)	44(1)	-4(1)	-2(1)	3(1)
C7	71(1)	48(1)	47(1)	7(1)	-6(1)	3(1)
C8	72(1)	58(1)	44(1)	8(1)	3(1)	-8(1)
C9	58(1)	58(1)	44(1)	1(1)	5(1)	-6(1)
C10	49(1)	56(1)	58(1)	10(1)	-2(1)	6(1)
C11	52(1)	47(1)	70(1)	8(1)	-9(1)	0(1)
C12	58(2)	72(2)	138(3)	34(2)	-23(2)	-4(1)
C13	51(1)	91(2)	81(2)	29(2)	6(1)	11(1)
C14	55(1)	59(1)	43(1)	-6(1)	-4(1)	1(1)
C15	56(2)	187(4)	160(3)	71(3)	22(2)	-7(2)
C16	98(2)	85(2)	134(3)	-34(2)	-45(2)	-6(2)
C17	62(1)	76(2)	58(1)	10(1)	-12(1)	9(1)
C18	61(4)	112(7)	97(6)	17(4)	-29(3)	14(4)
C18A	47(8)	67(8)	32(6)	10(5)	10(5)	-2(6)
N1	60(1)	61(1)	98(2)	5(1)	-24(1)	-7(1)
N2	43(1)	103(2)	120(2)	42(2)	2(1)	1(1)
O1	52(1)	57(1)	42(1)	7(1)	3(1)	2(1)
O2	63(1)	66(1)	57(1)	-12(1)	-9(1)	-5(1)
O3	63(1)	99(2)	205(3)	28(2)	-38(1)	-22(1)
O4	69(1)	148(2)	82(1)	14(1)	23(1)	25(1)
O5	55(1)	68(1)	54(1)	11(1)	-4(1)	9(1)

The anisotropic displacement factor takes the form:
 $\exp\{-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]\}$

Table 3b. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the non-hydrogen atoms of molecule B of the compound.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1'	79(2)	60(1)	70(1)	-25(1)	18(1)	-14(1)
C2'	79(1)	54(1)	52(1)	-9(1)	4(1)	-14(1)
C3'	59(1)	48(1)	53(1)	3(1)	3(1)	-1(1)
C4'	62(1)	47(1)	42(1)	1(1)	0(1)	5(1)
C5'	61(1)	48(1)	47(1)	-4(1)	3(1)	2(1)
C6'	61(1)	52(1)	63(1)	-6(1)	-6(1)	2(1)
C7'	84(2)	59(1)	64(1)	-16(1)	-17(1)	8(1)
C8'	90(2)	71(2)	53(1)	-17(1)	-4(1)	18(1)
C9'	68(1)	65(1)	51(1)	-3(1)	2(1)	14(1)
C10'	62(1)	55(1)	76(2)	-2(1)	-10(1)	-2(1)
C11'	96(2)	50(1)	99(2)	2(1)	-45(2)	-10(1)
C12'	87(2)	67(2)	259(6)	-39(3)	-69(3)	12(2)
C13'	57(1)	69(2)	126(2)	-16(2)	-2(2)	2(1)
C14'	126(2)	75(2)	49(1)	-2(1)	-6(1)	-27(2)
C15'	207(4)	83(2)	209(4)	29(3)	-149(4)	-6(2)
C16'	82(2)	166(4)	294(6)	-75(4)	46(3)	25(2)
C17'	55(2)	68(2)	71(3)	-19(2)	-1(2)	-5(2)
C17'B	127(1)	73(6)	68(8)	-15(6)	32(7)	0(6)
C18'	57(1)	94(3)	108(4)	-34(3)	9(2)	-20(2)
C18'B	86(1)	87(8)	160(1)	-14(9)	14(10)	16(7)
N1'	124(2)	59(1)	161(3)	-3(2)	-89(2)	2(2)
N2'	62(1)	85(2)	193(3)	-30(2)	-9(2)	11(1)
O1'	43(5)	42(6)	58(7)	-16(5)	7(5)	-5(4)
O1'B	73(5)	87(5)	74(5)	-34(3)	15(3)	-14(3)
O2'	143(2)	81(1)	75(1)	20(1)	-47(1)	-26(1)
O3'	103(2)	100(2)	363(5)	-43(2)	-102(2)	35(2)

The anisotropic displacement factor takes the form:
 $\exp\{-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]\}$

Table 4a. Atomic coordinates ($\times 10^4$) and their isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for hydrogen atoms of molecule A of the compound

Atom	x	y	z	U(iso)
H1A	5096	4564	991	59
H1B	4732	4903	1779	59
H2	6318	4940	1832	55
H3	6747	5168	633	57
H7	4441	7980	-992	66
H8	5990	7801	-1209	70
H9	6912	6858	-405	64
H14A	5606	6990	1832	62
H14B	5557	6229	2520	62
H15A	9693	6694	82	201
H15B	10286	7041	784	201
H15C	9733	7871	314	201
H15D	10115	7710	704	201
H15E	9522	7363	3	201
H15F	10075	6533	473	201

Table 4a. Continued

Atom	x	y	z	U(iso)
H16A	7737	7527	3153	159
H16B	8238	8508	2839	159
H16C	8809	7557	3141	159
H16D	8786	8201	2935	159
H16E	8284	7220	3250	159
H16F	7714	8171	2948	159
H17A	2907	7332	-876	79
H17B	3066	8354	-400	79
H18A	1542	7844	-342	136
H18B	2006	7785	460	136
H18C	1850	6765	-10	136
H18D	1520	7961	-413	73
H18E	1912	7906	414	73
H18F	1726	6878	-39	73

Table 4b. Atomic coordinates ($\times 10^4$) and their isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for hydrogen atoms of molecule B of the compound

Atom	x	y	z	U(iso)
H1'A	2999	7521	-2447	84
H1'B	3266	7997	-3222	84
H2'	1680	7942	-3091	74
H3'	1512	8168	-1835	64
H7'	3878	11206	-571	83
H8'	2352	11181	-301	85
H9'	1353	10138	-965	74
H14'A	2362	9996	-3188	100
H14'B	2235	9240	-3874	100
H15'A	75	10908	-4037	253
H15'B	-750	11495	-3680	253
H15'C	-914	10439	-4104	253
H15'D	-1134	10987	-3844	253
H15'E	-309	10400	-4201	253
H15'F	-145	11456	-3777	253
H16'A	-1861	9292	-1280	270
H16'B	-1841	10508	-1354	270
H16'C	-1162	9945	-794	270
H16'D	-1381	10538	-1005	270
H16'E	-1402	9322	-931	270
H16'F	-2080	9885	-1492	270
H17'A	5224	10512	-603	78
H17'B	5156	11465	-1160	78
H17'C	5889	10874	-2003	107
H17'D	5300	11605	-1475	107
H18'A	6680	10912	-1050	129
H18'B	6321	10742	-1878	129
H18'C	6391	9797	-1322	129
H18'D	6442	10782	-780	166

Table 5a. Torsion angles (°) of molecule A of the compound

Atoms	Angle (°)	Atoms	Angle (°)
C1-C2-C14-O2	177.6(1)	C10-C11-O2-C14	-9.7(3)
C1-C2-C3-C10	166.6(1)	C10-C13-N2-C12	7.0(4)
C1-C2-C3-C4	41.2(2)	C10-C13-N2-C15	-173.4(2)
C2-C14-O2-C11	41.2(2)	C10-C3-C4-C5	-132.2(2)
C2-C1-O1-C5	51.1(2)	C10-C3-C4-C9	48.3(2)
C2-C3-C10-C11	-16.7(2)	C11-C10-C13-N2	-7.4(3)
C2-C3-C10-C13	155.9(2)	C11-C10-C13-O4	173.4(2)
C2-C3-C4-C5	-10.0(2)	C13-C10-C11-N1	3.0(3)
C2-C3-C4-C9	170.5(2)	C13-C10-C11-O2	-175.4(2)
C3-C10-C11-N1	175.7(2)	C14-C2-C3-C10	45.8(2)
C3-C10-C11-O2	-2.7(3)	C14-C2-C3-C4	-79.7(2)
C3-C10-C13-N2	179.9(2)	C18-C17-O5-C6	179.8(5)
C3-C10-C13-O4	0.6(4)	C18A-C17-O5-C6	-178.1(8)
C3-C2-C14-O2	-60.5(2)	N1-C11-O2-C14	171.71(2)
C3-C4-C5-C6	175.9(2)	N1-C12-N2-C13	-1.6(4)
C3-C4-C5-O1	-2.3(3)	N1-C12-N2-C15	178.8(2)
C3-C4-C9-C8	-177.5(2)	N2-C12-N1-C11	-3.4(3)
C4-C3-C10-C11	106.4(2)	N2-C12-N1-C16	-178.8(2)
C4-C3-C10-C13	-81.1(2)	O1-C1-C2-C3	-63.7(2)
C4-C5-C6-C7	2.8(3)	O1-C1-C2-C14	57.8(2)
C4-C5-C6-O5	-177.8(2)	O1-C5-C6-C7	-178.7(2)
C4-C5-O1-C1	-18.7(2)	O1-C5-C6-O5	0.7(2)
C5-C4-C9-C8	3.0(3)	O2-C11-N1-C12	-178.6(2)
C5-C6-C7-C8	0.6(3)	O2-C11-N1-C16	-3.4(3)
C5-C6-O5-C17	-176.78(2)	O3-C12-N1-C11	176.6(2)
C6-C5-O1-C1	162.9(1)	O3-C12-N1-C16	1.2(4)
C6-C7-C8-C9	-2.1(3)	O3-C12-N2-C13	178.4(2)
C7-C6-O5-C17	2.7(3)	O3-C12-N2-C15	-1.2(4)
C7-C8-C9-C4	0.3(3)	O4-C13-N2-C12	-173.7(2)
C9-C4-C5-C6	-4.5(3)	O4-C13-N2-C15	5.9(4)
C9-C4-C5-O1	177.2(1)	O5-C6-C7-C8	-178.8(2)
C10-C11-N1-C12	2.7(3)		
C10-C11-N1-C16	177.9(2)		

Table 5b. Torsion angle of molecule B of the compound

Atoms	Angle (°)	Atoms	Angle (°)
C1'-C2'-C14'-O2'	-178.5(2)	C10'-C11'-O2'-C14'	-6.9(4)
C1'-C2'-C3'-C10'	171.4(2)	C10'-C13'-N2'-C12'	3.2(4)
C1'-C2'-C3'-C4'	47.0(2)	C10'-C13'-N2'-C16'	-172.1(3)
C2'-C14'-O2'-C11'	35.3(3)	C10'-C3'-C4'-C5'	-142.1(2)
C2'-C1'-O1'-B-C5'	43.7(1)	C10'-C3'-C4'-C9'	37.3(3)
C2'-C1'-O1'-C5'	33.0(2)	C11'-C10'-C13'-N2'	-6.6(3)
C2'-C3'-C10'-C11'	-23.1(3)	C11'-C10'-C13'-O4'	173.7(3)
C2'-C3'-C10'-C13'	153.6(2)	C13'-C10'-C11'-N1'	3.3(4)
C2'-C3'-C4'-C5'	-19.5(3)	C13'-C10'-C11'-O2'	-175.7(2)
C2'-C3'-C4'-C9'	159.9(2)	C14'-C2'-C3'-C10'	48.7(2)
C3'-C10'-C11'-N1'	-180.0(2)	C14'-C2'-C3'-C4'	-75.6(2)
C3'-C10'-C11'-O2'	1.0(4)	C18'B-C17'B-O5'-C17'	38.6(1)
C3'-C10'-C13'-N2'	176.6(2)	C18'B-C17'B-O5'-C6'	100.8(1)
C3'-C10'-C13'-O4'	-3.1(4)	C18'-C17'-O5'-C17'B	-49.4(1)

Table 5b. Continued

Atoms	Angle (°)	Atoms	Angle (°)
C3'-C2'-C14'-O2'	-56.7(2)	C18'-C17'-O5'-C6'	174.0(2)
C3'-C4'-C5'-C6'	179.1(2)	N1'-C11'-O2'-C14'	3.6(5)
C3'-C4'-C5'-O1'	-4.3(2)	N1'-C12'-N2'-C13'	178.9(3)
C3'-C4'-C5'-O1'B	1.9(7)	N1'-C12'-N2'-C16'	-7.3(4)
C3'-C4'-C9'-C8'	-179.3(2)	N2'-C12'-N1'-C11'	-178.1(3)
C4'-C3'-C10'-C11'	99.6(2)	N2'-C12'-N1'-C15'	60.5(7)
C4'-C3'-C10'-C13'	-83.7(2)	O1'B-C1'-C2'-C14'	64.9(12)
C4'-C5'-C6'-C7'	0.7(3)	O1'-C1'-C2'-C14'	-60.9(7)
C4'-C5'-C6'-O5'	179.7(2)	O1'B-C1'-C2'-C3'	-56.6(1)
C4'-C5'-O1'B-C1'	-14.2(1)	O1'-C1'-C2'-C3'	83(2)
C4'-C5'-O1'-C1'	-2(2)	O1'B-C1'-O1'-C5'	-88(2)
C5'-C4'-C9'-C8'	0.1(3)	O1'-C1'-O1'B-C5'	178.0(6)
C5'-C6'-C7'-C8'	-0.7(3)	O1'B-C5'-C6'-C7'	-176.4(1)
C5'-C6'-O5'-C17'	-173.7(3)	O1'-C5'-C6'-C7'	-3.0(6)
C5'-C6'-O5'-C17'B	154.0(9)	O1'B-C5'-C6'-O5'	2.5(1)
C6'-C5'-O1'B-C1'	168.6(7)	O1'-C5'-C6'-O5'	-50(1)
C6'-C5'-O1'-C1'	174.9(12)	O1'B-C5'-O1'-C1'	121(1)
C6'-C7'-C8'-C9'	0.4(4)	O1'-C5'-O1'B-C1'	-176.8(3)
C7'-C6'-O5'-C17'	5.2(4)	O2'-C11'-N1'-C12'	-6.1(3)
C7'-C6'-O5'-C17'B	-27.1(9)	O2'-C11'-N1'-C15'	174.6(3)
C7'-C8'-C9'-C4'	-0.1(3)	O3'-C12'-N1'-C11'	3.8(5)
C9'-C4'-C5'-C6'	-0.4(3)	O3'-C12'-N1'-C15'	-178.4(3)
C9'-C4'-C5'-O1'	176.3(4)	O3'-C12'-N2'-C13'	-3.0(5)
C9'-C4'-C5'-O1'B	-177.6(6)	O3'-C12'-N2'-C16'	-177.1(3)
C10'-C11'-N1'-C12'	4.1(4)	O4'-C13'-N2'-C12'	7.6(4)
C10'-C11'-N1'-C15'	174.7(2)	O4'-C13'-N2'-C16'	-179.6(2)
		O5'-C6'-C7'-C8'	

ering parameters (Cremer & Pople, 1975) $q_2 = 0.377(2)$ Å, $\Phi_2 = 159.3(3)^\circ$ for pyran and $q_2 = 0.392(2)$ Å, $\Phi_2 = 23.55(3)^\circ$ for pyran ring of the chromene moiety. Similarly with puckering parameter $q_2 = 0.355(3)$ Å, $\Phi_2 = 169.9(2)^\circ$ the pyran ring of molecule B assumes sofa conformations. It could be further confirmed from the least-square planes analysis, the atoms (C2 and C2') are found to be deviated by maximum deviation of $-0.297(2)$ Å and $0.292(2)$ Å from other atoms, with indicate the atoms C2 and C2' at the flap of the sofa in molecules A and B, respectively.

The partial double bond character of bonds surrounded by the nitrogen atoms C11-N1 [1.382(3) Å], N1-C12 [1.374(4) Å], C12-N2 [1.373(4) Å] and N2-C13 [1.416(4) Å], shows a high degree of electron delocalization in the molecule A. Similarly the bonds surrounded by the nitrogen atoms C11'-N1' [1.393(4) Å], N1'-C12' [1.377(6) Å], C12'-N2' [1.362(6) Å] and N2'-C13' [1.400(4) Å], shows a high degree of electron delocalization in the molecule B.

5. Conclusion

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 5%. There are two independent molecules present in the asymmetric unit. In general the chromene derivatives are well characterized in terms 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. 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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