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) Å and c= 17.781(4) Å [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 possess several biological and pharmacological properties such as anti-coagulant, anti-sterility, antiviral, anti-fungal, anti-inflammatory, cardiont honic, anti-diabetic, spasmyltic, diuretic, anti-anaphylactic, anti-cancer activities[3-12] and also useful in treatment of Schizophrenia and Alzheimer’s disease[13,14]. Recently, the structural modification of chromene scaffold with the addition of heterocyclic substituents 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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(Received: January 24, 2015, Revised: March 16, 2015, Accepted: March 25, 2015)
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 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 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_{2}O_{5} was used for data collection on a Bruker Kappa APEX II CCD diffractometer\(^\text{[15]}\). The MoK\(^\alpha\) radiation of wavelength, (\(\lambda = 0.71073 \text{ Å}\)) 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\(^\text{[16,17]}\). 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\(^\text{[18]}\) and PLATON\(^\text{[19]}\). The software used to prepare material for publication is WinGX publication routines\(^\text{[20]}\). 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_{22}H_{18}N_{2}O_{5} |
| **Formula weight** | 344.36 |
| **Temperature** | 293(2) K |
| **Wavelength** | 0.71073 Å |
| **Crystal system** | Monoclinic |
| **space group** | P2\(_1\)/c |
| **Unit cell dimensions** | |
| | \(a = 14.608 \text{ (3) Å}\) |
| | \(b = 12.845 \text{ (3) Å}\) |
| | \(c = 17.781 \text{ (4) Å}\) |
| | \(\beta = 91.233 \text{ (5)°}\) |
| **Volume** | 3355.7 (12) Å\(^3\) |
| **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 |
| **Completeness to theta** | [Rint = 0.039] |
| **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>2σ(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\(^{-3}\) |
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
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 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)°. 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 127command 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 (Å²×10³) for the non-hydrogen atoms of molecule A of the compound.

| Atom  | U₁₁  | U₂₂  | U₃₃  | U₁₂  | U₁₃  | U₂₃  |
|-------|------|------|------|------|------|------|
| 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:

\[\exp\{-2\pi^2 [h^2a^*^2U_{11}+...+2hk a^* b^* U_{12}]\}\]
Table 3b. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for the non-hydrogen atoms of molecule B of the compound.

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|------|----------|----------|----------|----------|----------|----------|
| 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()     | 94(3)    | 108(4)   | -34(3)   | 9(2)     | -20(2)   |

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

Table 4a. Atomic coordinates ($\times 10^4$) and their isotropic displacement parameters ($\text{Å}^2 \times 10^3$) 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    |

J. Chosun Natural Sci., Vol. 8, No. 1, 2015
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 | 10   | 136    |
| H18E  | 1912 | 7906 | 414  | 73     |
| H18F  | 1726 | 6878 | -39  | 73     |

Table 4b. Atomic coordinates ($\times 10^4$) and their isotropic displacement parameters ($\AA^2 \times 10^3$) 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| 6591 | 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-C14-O2-C11           | 51.1(2)   | C10-C3-C4-C9               | 48.3(2)   |
| C2-C1-C14-O2-C11           | -16.7(2)  | C10-C14-C13-C12            | -7.4(3)   |
| C2-C1-C14-O2-C11           | 155.9(2)  | C11-C10-C13-O4             | 173.4(2)  |
| C2-C3-C4-C5               | -10.8(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-C4               | 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              | 171.7(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-C4               | 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-C4-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'-C15'-O1'-C5'           | 43.7(1)   | C10'-C3'-C4'-C9'          | 37.3(3)   |
| C2'-O1'-C15'-C3'           | 33.0(2)   | C11'-C10'-C13'-N2'        | -6.6(3)   |
| C2'-C3'-C10'-O1'-C14'      | -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'-C14'    | -180.0(2) | C14'-C2'-C3'-C4'          | -75.6(2)  |
| C3'-C10'-C11'-O2'          | 1.0(4)    | C18'-C17'-O5'-C17'        | 38.6(1)   |
| C3'-C10'-C13'-N2'          | 176.6(2)  | C18'-C17'-O5'-C6'         | 100.8(1)  |
| C3'-C10'-C13'-O4'          | -3.1(4)   | C18'-C17'-O5'-C17'B       | -49.4(1)  |

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ering parameters (Cremer & Pople, 1975) \( q_2 = 0.377(2) \) Å, \( \Phi_2 = 159.3(3)° \) for pyran and \( q_2 = 0.392(2) \) Å, \( \Phi_2 = 23.55(3)° \) for pyran ring of the chromene moiety. Similarly with puckering parameter \( q_2 = 0.355(3) \) Å, \( \Phi_2 = 169.9(2)° \) 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.

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(3)  | 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'C1'-N1'-C12'       | -6.1(3)   |
| C7'-C6'-O5'-C17'B     | -27.1(9)  | O2'C1'-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) |

Table 5b. Continued

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 molecule 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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Acknowledgement

The authors thank the Technology Business Incubator facility at University of Madras, Chennai.

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