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Crystal and Molecular Structure Analysis of Diethyl-Dithiocarbamic Acid 6-methyl-2-oxo-2H-chromen-4-ylmethyl ester

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Abstract: ***The crystal and molecular structure of Diethyl-dithiocarbamic acid 6-methyl-2-oxo-2H-chromen-4-ylmethyl ester is described. The compound crystallizes in the monoclinic space group P21/c with a = 7.8105(11)Å, b = 7.9975(11)Å, c = 25.198(4)Å, β = 98.753(2) °, V = 1555.7(4)Å3, z= 4. The crystal structure is stabilized by intermolecular C–H…N, C–H…S, C-H... O, C–H…π and π-π stacking interactions.***

Keywords: C–H…N, C–H…S, C-H... O, C–H…π and π-π stacking intermolecular interactions; crystal structure; coumarin derivative

1. Introduction

Coumarins and their derivatives have attracted considerable attention due to their extensive biological activities such as antibacterial, antifungal, antiviral, anti-tubercular, anti-malarial, anticoagulant, anti-inflammatory, anticancer, antioxidant properties [1]. Numerous efforts including the separation and purification of naturally occurring coumarins from a variety of plants as well as artificial synthesis of coumarin compounds with novel structures and properties have been the focus of research and development for potential drugs [2]. So far, some coumarins, for example, warfarin, acenocoumarol, armillarisin A [3], hymecromone and carbochromen have been approved for therapeutic purposes in clinic [4].

Synthetic coumarin derivatives have been obtained by chemical modification of the coumarin ring. More importantly, an increasing number of synthetic coumarin compounds have displayed great potency in the treatment of various types of diseases [5].

Coumarins have outstanding optical properties, including an extended spectral range, high quantum yields, superior photostability and good solubility in common solvents. So, these compounds are widely used as laser dyes [6] nonlinear optical chromophores [7], fluorescent whiteners [8], as well as fluorescent labels and probes for physiological measurement [9]. Another feature of the coumarin derivatives is that photophysical and spectroscopic properties can be readily modified by the introduction of substituents in the coumarin ring, giving themselves more flexibility to fit well in various applications [10]. Coumarin derivatives have attracted much attention due to their potential application for OLEDs [11]. Coumarins, chromones and flavones are widely distributed edible plant products, some of which are known to inhibit the induction of tumors by carcinogenic chemicals [12].

The crystal structure analyses of coumarin derivatives reveal several structural aspects which have attracted intense interest in recent years, because of their diverse pharmacological properties. Coumarins, an old class of compounds, are naturally occurring benzopyrone derivatives. The pharmacological, biochemical properties and therapeutic applications of simple coumarins depend upon the pattern of substitution. These include the latent structural asymmetry, the substituted methyl group at C_6 with respect to the coumarin ring, the diethyl-dithiocarbamic acid substitution at C_4. Additionally, these compounds provide essential molecular frameworks that predispose them to biological activity [13].

The title compound being a derivative of coumarin possessed wide-ranging biological properties. In addition to biological activities associated with 4-substituted coumarins, the groups linked at the C-4 methylene carbon have profound influence on their solid-state conformations. A single crystal X-ray diffraction analysis was carried out to establish the crystal as well as molecular structure and to understand the self-aggregation in terms of possible intermolecular interactions.

2. Experimental

The compound was prepared according to the reported method [14]. A mixture of diethyl dithiocarbamic acid **2** (1.53g, 10 mmol) and anhydrous potassium carbonate (1.38g, 10mmol) was stirred for 30 min in dry acetone (30 mL). To this, 4-bromomethyl-6-methyl-chromen-2-one **1** (2.67g, 10 mmol) was added and the stirring was continued for 24h. Then, the resulting reaction mixture was poured to crushed ice. The separated solid was filtered and washed with 1: 1 HCl (30 mL) and water. Then product **3** was recrystallised from ethanol to get pale yellow needles. Colourless blocks of the title compound were grown from a mixed solution of EtOH/$CHCl_3$ (V/V = 2/1) by slow

evaporation at room temperature. Yield was 90%, melting point 155^0 C.

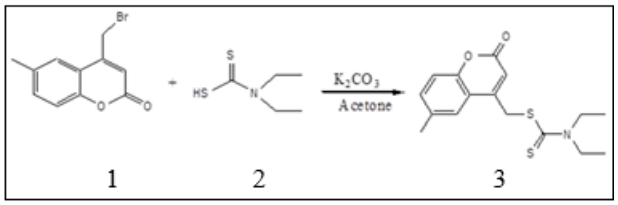


Figure 1

Table 1.1: Summary of crystal data, intensity data collection and refinement of compound 3

Crystal data	
$C_{16}H_{19}NO_2S_2$	$D_x = 1.372 Mgm^{-3}$
$M_r = 321.44$	Mo Kα radiation 0.71073 Å
Monoclinic, $P2_1/c$	$\theta = 2.64 - 27.00°$
$a = 7.8105(11)$Å	$\mu = 0.346 mm^1$
$b = 7.9975(11)$Å	$T = 293$ (2) K
$c = 25.198(4)$Å	Needle, pale yellow
$\beta = 98.753(2)°$	0.18 × 0.16 × 0.16 mm
$V = 1555.7(4)$Å^3	
$Z = 4$	
Data collection	
Bruker SMART CCD area - detector diffractometer	2763 reflections with I > 2σ(I)
φ and ω scans	$R_{int} = 0.0812$
Absorption correction: none	$\theta_{max} = 27.0°$
9079 measured reflections	h = -9→ 9
3392 independent reflections	k = -7 → 10
	l = -32 → 31
Refinement	
Refinement on F^2	$w = 1/[\sigma^2(Fo^2) + (0.1797P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.0632$	+3.4500P]
$wR(F^2) = 0.2109$	where $P = (Fo^2 + 2Fc^2)/3$
S = 0.795	$(\Delta/\sigma)_{max} = 0.001$
3392 reflections	$\Delta\rho_{max} = 0.779$ e Å^{-3}
193 parameters	$\Delta\rho_{min} = -0.791$ e Å^{-3}
H-atom parameters constrained	

Programs used

Data collection:	SMART (Bruker, 1998);
Cell refinement:	SMART;
Data reduction:	SAINT (Bruker, 1998);
Structure solution:	SHELXS97 (Sheldrick, 2008);
Structure refinement:	SHELXL97 (Sheldrick, 2008);
Molecular graphics:	PLUTON (Speck, 1997); ORTEP-3 (Farrugia, 1997); CAMERON (Watkin et al., 1993); WinGX (Farrugia, 1999)

X-Ray Structure Analysis

The X-ray diffraction data for compound 3 were collected on a Bruker Smart CCD Area Detector System (IISc, Bangalore), using MoKαω (0.71073Å) radiation for the crystal. Intensity data were collected up to a max of 27.00° for the compound in the ω–ϕ scan mode. The data were reduced using SAINT [15]. A total of 9079 reflections were collected, resulting in 3392 independent reflections of which the number of reflections satisfying I>2 σ(I) criteria were 2763. These were treated as observed. It was confirmed that the crystal belongs to monoclinic crystal system and the space group is $P2_1/c$. The structure was solved by direct methods and difference Fourier synthesis using SHELXS97[16]. The positions of all non-hydrogen atoms were included in the full-matrix least-square refinement using SHELXL97. Anisotropic refinement using full-matrix least-square procedures was carried out for a few cycles until convergence was reached. All hydrogen atoms were located in difference Fourier maps and refined isotropically. The H atoms were placed at calculated positions in the riding model approximation (C—H 0.93Å); their temperature factors were set to 1.2 times those of the equivalent isotropic temperature factors of the parent atoms. All other non-H atoms were refined anisotropically. The R factor after final convergence was 0.0632 and the maximum and minimum values of residual electron density were 0.779 and –0.791 eÅ^{-3}. Molecular diagrams were generated using ORTEP [17]. The mean plane calculation was done using the program PARST [18].

3. Results and Discussion

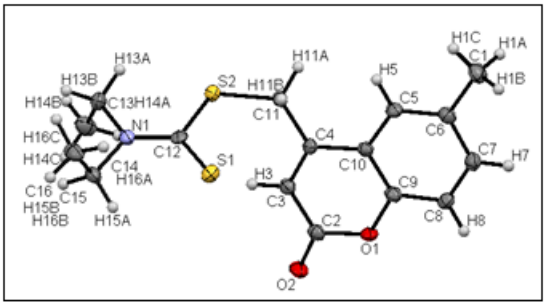


Figure 1.1: ORTEP diagram of compound 3, showing 50% probability displacement ellipsoids and the atom-numbering scheme. An intramolecular C–H…S hydrogen bond.

Figure 1.1 shows the ORTEP diagram of title compound. Table 1.1 summarizes the crystal data, intensity data collection and refinement details for the compound 3. The atomic coordinates of the nonhydrogen atoms with their equivalent temperature factors for the compound are presented in Table 1.2. Anisotropic displacement parameters are given in Table 1.3. The corresponding bond lengths and angles are given in Tables 1.4. The torsion angles for the nonhydrogen atoms are listed in Table 1.5. Table 1.6 shows the atomic coordinates and isotropic displacement parameters for the hydrogen atoms. The least-squares planes calculated using the programs PARST [18] are tabulated in Table 1.7. The intra- and intermolecular hydrogen bonds including the weak interactions are listed in Table 1.9.

The compound crystallizes in space group $P2_1/c$. In the title molecule, an intramolecular C–H…S hydrogen bond (Fig 1.1) forms a pseudo-seven-membered ring with graph set S(7), thus locking the molecular conformation and eliminating conformational flexibility. The two rings in the molecule are nearly coplanar. The dihedral angle between the least-squares plane of the phenyl and pyrone rings is 1.28(7)°Table-1.8, confirming the planarity of the coumarin moiety. The bond lengths and bond angles in the coumarin moiety of the molecule show a fair amount of agreement with some 4-substituted coumarin derivatives [19]. The heterocyclic ring is distorted by about 5º, but the phenylene moiety is nearly planar. The orientation of methyl ester group is characterized by torsion angles C(4)-C(11)-S(2)-C (12) of 80.2(2) ° (Table 1.5). The survey of the structure at a molecular level reveals usual geometrical parameters for the S–C bond of 1.785(3)Å (Table 1.4).

Intermolecular Features

The packing of layers of molecules is stabilized by the presence of an intermolecular short contact of types C-H…O, C-H…N and C-H…S. The C-H…O interaction generates centrosymmetric head-to-head dimers with packing motifs in accordance with Etter's analysis are $R^2_2(8)$

along the crystallographic '*b*'-axis. The C-H…S interaction also forms dimers corresponding to graph set notation $R^2_2(22)$ [20] along 'a' axis (Fig. 1.2).

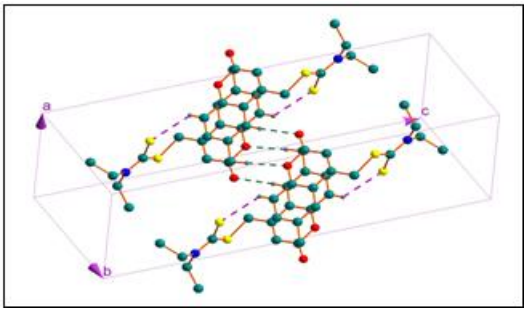


Figure 1.2: C-H...O and C–H…S dimers in 3 along crystallographic 'a' and 'b'-axes

The C-H...O and C-H...N interactions links the molecules into chains along the crystallographic '*a*'-axis (Fig. 1.3). Weak C–H…π intermolecular interactions further stabilizes the packing of the molecules in the crystal lattice (Fig. 1.5). The C–H…π interactions involve the coumarin ring and the phenyl ring. The packing of layers of molecules is further stabilized by π-π stacking interactions (Fig. 1.4) between the pyrone and phenyl ring with a shortest centroid-centroid distance of 3.718Å. The supramolecular aggregation in this structure is due to C–H…N, C–H…S, C-H...O, C–H…π and π-π stacking intermolecular interactions.

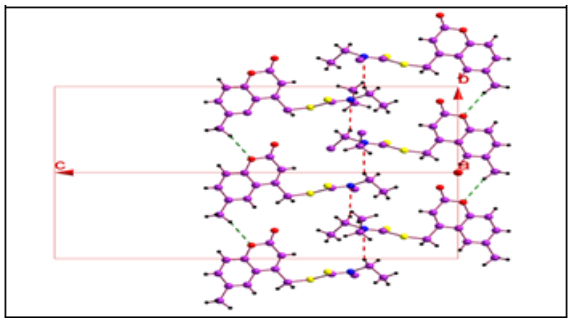


Fig. 1.3: C-H...O and C–H…N dimers in 3 along crystallographic 'a'-axis

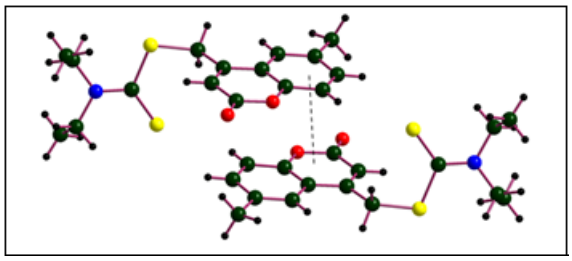


Fig: 1.4: A π-π interaction in 3 along 'b' axis

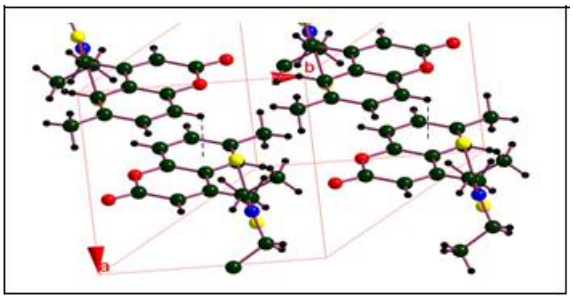


Fig. 1.5: C–H…π interaction in 3 along 'c'-axis

Table 1.2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2× 10^3) of compound 3

Atom	x	y	z	U(eq)
C(1)	4869(4)	5120(4)	5913(1)	29(1)
C(2)	1533(4)	11825(4)	4668(1)	20(1)
C(3)	815(4)	10364(3)	4377(1)	19(1)
C(4)	1268(4)	8787(3)	4533(1)	18(1)
C(5)	3080(4)	6959(4)	5225(1)	20(1)
C(6)	4278(4)	6815(4)	5689(1)	20(1)
C(7)	4954(4)	8282(4)	5946(1)	23(1)
C(8)	4422(4)	9857(4)	5754(1)	20(1)
C(9)	3204(4)	9966(4)	5293(1)	20(1)
C(10)	2520(4)	8536(3)	5014(1)	17(1)
C(11)	558(4)	7258(3)	4224(1)	20(1)
C(12)	32(4)	8219(3)	3135(1)	19(1)
C(13)	−2856(4)	8089(4)	2564(1)	23(1)
C(14)	−3996(4)	9606(4)	2612(1)	31(1)
C(15)	−291(4)	9150(4)	2198(1)	22(1)
C(16)	331(5)	7798(4)	1848(1)	29(1)
O(1)	2719(3)	11555(2)	5124(1)	20(1)
O(2)	1184(3)	13272(2)	4551(1)	25(1)
N(1)	−993(3)	8467(3)	2665(1)	19(1)
S(1)	2175(1)	8465(1)	3230(1)	21(1)
S(2)	−1118(1)	7577(1)	3660(1)	19(1)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}(a_i^* a_j^*)(a_i.a_j)$

Table 1.3: Anisotropic displacement parameters (Å^2×10^3) of 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}\,]$

Atom	U11	U22	U33	U23	U13	U12
C(1)	33(2)	25(2)	28(2)	5(1)	−1(1)	5(1)
C(2)	24(2)	19(1)	17(1)	1(1)	6(1)	0(1)
C(3)	23(1)	17(1)	17(1)	1(1)	3(1)	1(1)
C(4)	22(1)	17(1)	14(1)	−1(1)	4(1)	−2(1)
C(5)	27(2)	14(1)	18(1)	−2(1)	4(1)	−1(1)
C(6)	22(2)	20(1)	19(1)	2(1)	6(1)	1(1)
C(7)	27(2)	23(2)	17(1)	0(1)	2(1)	0(1)
C(8)	21(1)	20(1)	19(1)	−4(1)	2(1)	−2(1)
C(9)	25(1)	15(1)	18(1)	0(1)	5(1)	1(1)
C(10)	21(1)	16(1)	15(1)	0(1)	6(1)	−1(1)
C(11)	29(2)	15(1)	14(1)	1(1)	2(1)	0(1)
C(12)	25(1)	10(1)	21(1)	−4(1)	0(1)	−1(1)
C(13)	23(2)	24(1)	20(1)	2(1)	−3(1)	−4(1)
C(14)	23(2)	30(2)	39(2)	10(1)	4(1)	2(1)
C(15)	29(2)	18(1)	18(1)	4(1)	4(1)	0(1)
C(16)	47(2)	19(1)	22(1)	−1(1)	9(1)	−1(1)
O(1)	26(1)	11(1)	21(1)	−1(1)	2(1)	−2(1)
O(2)	36(1)	13(1)	24(1)	2(1)	1(1)	1(1)
N(1)	25(1)	15(1)	17(1)	−1(1)	3(1)	−1(1)
S(1)	21(1)	21(1)	22(1)	−3(1)	2(1)	−2(1)
S(2)	21(1)	18(1)	16(1)	−1(1)	1(1)	−2(1)

Table 1.4: Bond lengths [Å] and angles [°] for non-H-atoms of 3 with esds in parenthesis

C(1)-C(6)	1.513(4)
C(2)-O(2)	1.215(4)
C(2)-O(1)	1.379(3)
C(2)-C(3)	1.446(4)
C(3)-C(4)	1.352(4)
C(4)-C(10)	1.450(4)
C(4)-C(11)	1.510(4)
C(5)-C(6)	1.386(4)
C(5)-C(10)	1.412(4)
C(6)-C(7)	1.404(4)
C(7)-C(8)	1.390(4)
C(8)-C(9)	1.387(4)
C(9)-O(1)	1.375(3)
C(9)-C(10)	1.405(4)
C(11)-S(2)	1.798(3)
C(12)-N(1)	1.339(4)
C(12)-S(1)	1.666(3)
C(12)-S(2)	1.785(3)
C(13)-N(1)	1.469(4)
C(13)-C(14)	1.520(4)
C(15)-N(1)	1.476(4)
C(15)-C(16)	1.521(4)
O(2)-C(2)-O(1)	116.7(3)
O(2)-C(2)-C(3)	126.3(3)
O(1)-C(2)-C(3)	117.1(2)

C(4)-C(3)-C(2)	122.9(2)
C(3)-C(4)-C(10)	119.0(2)
C(3)-C(4)-C(11)	123.1(2)
C(10)-C(4)-C(11)	117.8(2)
C(6)-C(5)-C(10)	121.5(3)
C(5)-C(6)-C(7)	118.6(3)
C(5)-C(6)-C(1)	121.1(3)
C(7)-C(6)-C(1)	120.3(3)
C(8)-C(7)-C(6)	121.6(3)
C(9)-C(8)-C(7)	118.6(3)
O(1)-C(9)-C(8)	116.0(2)
O(1)-C(9)-C(10)	122.1(2)
C(8)-C(9)-C(10)	121.9(3)
C(9)-C(10)-C(5)	117.8(3)
C(9)-C(10)-C(4)	117.5(2)
C(5)-C(10)-C(4)	124.7(2)
C(4)-C(11)-S(2)	117.31(19)
N(1)-C(12)-S(1)	124.2(2)
N(1)-C(12)-S(2)	113.4(2)
S(1)-C(12)-S(2)	122.36(17)
N(1)-C(13)-C(14)	113.5(2)
N(1)-C(15)-C(16)	112.9(2)
C(9)-O(1)-C(2)	121.4(2)
C(12)-N(1)-C(13)	124.4(2)
C(12)-N(1)-C(15)	120.9(2)
C(13)-N(1)-C(15)	114.6(2)
C(12)-S(2)-C(11)	103.82(14)

Esds: Estimated standard deviations

Table 1.5: Torsion angles [°] for non-H-atoms of 3 with esds in parenthesis

O(2)-C(2)-C(3)-C(4)	-179.9(3)
O(1)-C(2)-C(3)-C(4)	-0.4(4)
C(2)-C(3)-C(4)-C(10)	0.3(4)
C(2)-C(3)-C(4)-C(11)	-178.4(3)
C(10)-C(5)-C(6)-C(7)	-0.8(4)
C(10)-C(5)-C(6)-C(1)	179.9(3)
C(5)-C(6)-C(7)-C(8)	1.5(4)
C(1)-C(6)-C(7)-C(8)	-179.2(3)
C(6)-C(7)-C(8)-C(9)	-0.6(4)
C(7)-C(8)-C(9)-O(1)	179.5(3)
C(7)-C(8)-C(9)-C(10)	-1.0(4)
O(1)-C(9)-C(10)-C(5)	-179.0(2)
C(8)-C(9)-C(10)-C(5)	1.6(4)
O(1)-C(9)-C(10)-C(4)	0.1(4)
C(8)-C(9)-C(10)-C(4)	-179.4(3)
C(6)-C(5)-C(10)-C(9)	-0.7(4)
C(6)-C(5)-C(10)-C(4)	-179.7(3)
C(3)-C(4)-C(10)-C(9)	-0.2(4)
C(11)-C(4)-C(10)-C(9)	178.6(2)
C(3)-C(4)-C(10)-C(5)	178.9(3)
C(11)-C(4)-C(10)-C(5)	-2.4(4)
C(3)-C(4)-C(11)-S(2)	-6.1(4)
C(10)-C(4)-C(11)-S(2)	175.2(2)
C(8)-C(9)-O(1)-C(2)	179.3(2)
C(10)-C(9)-O(1)-C(2)	-0.2(4)
O(2)-C(2)-O(1)-C(9)	179.9(3)
C(3)-C(2)-O(1)-C(9)	0.4(4)
S(1)-C(12)-N(1)-C(13)	173.4(2)
S(2)-C(12)-N(1)-C(13)	-6.2(3)
S(1)-C(12)-N(1)-C(15)	-6.0(4)
S(2)-C(12)-N(1)-C(15)	174.34(19)
C(14)-C(13)-N(1)-C(12)	97.7(3)
C(14)-C(13)-N(1)-C(15)	-82.8(3)
C(16)-C(15)-N(1)-C(12)	90.5(3)
C(16)-C(15)-N(1)-C(13)	-89.1(3)
N(1)-C(12)-S(2)-C(11)	177.7(2)
S(1)-C(12)-S(2)-C(11)	-2.0(2)
C(4)-C(11)-S(2)-C(12)	80.2(2)

Table 1.6: Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2×10^3) of 3

Atom	x	y	z	U(eq)
H(1A)	4372	4906	6232	44
H(1B)	6110	5108	5998	44
H(1C)	4501	4273	5650	44
H(3)	7	10516	4070	23
H(5)	2636	5995	5048	24
H(7)	5778	8198	6253	27
H(8)	4873	10818	5930	24
H(11A)	112	6506	4473	23
H(11B)	1515	6692	4096	23
H(13A)	-3107	7244	2818	28
H(13B)	-3144	7625	2206	28
H(14A)	-3761	10040	2971	46
H(14B)	-5192	9285	2533	46
H(14C)	-3754	10450	2363	46
H(15A)	669	9890	2325	26
H(15B)	-1181	9808	1982	26
H(16A)	1291	7213	2049	43
H(16B)	691	8302	1538	43
H(16C)	-595	7026	1737	43

Table 1.7: Mean planes through various groups of atoms and deviations (Å) from the plane in 3. The equation of the plane: m1X+m2Y+m3Z-D = 0 where m1, m2, m3 and D are constant. Starred atoms are included in the plane calculations

Plane	m1	m2	m3	D	Atom	Deviations
1	0.833(9)	0.017(7)	-0.551(9)	-6.736(5)	C2*	-0.0034(3)
					C3*	0.0005(2)
					C4*	0.0093(2)
					C10*	0.0077(2)
					C5*	-0.0072(3)
					C6*	-0.0149(3)
					C7*	0.0099(3)
					C8*	0.0115(3)
					C9*	0.0003(2)
					O1*	-0.0072(2)

Table 1.8: Dihedral angles formed by LSQ-Planes in 3.

Plane1	Plane2	Angle
Phenyl ring	Pyrone ring	1.28(7)°

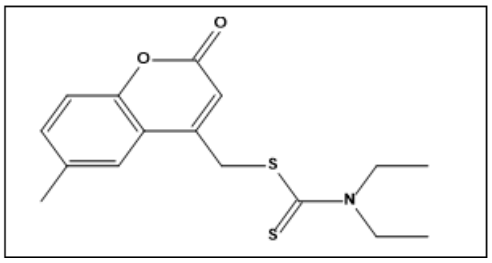
Table 1.9: Nonbonded interactions and possible hydrogen bonds in 3 (Å, °). *(D-donor; A-Acceptor; H-hydrogen)*

D–H...A	D–H	H...A	D...A	D–H...A
C3–H3···S2	0.930 (3)	2.662(1)	3.112 (3)	110(2)
C8–H8···S1^{i}	0.930(3)	2.939(1)	3.654(3)	135(2)
C5–H5···O1^{ii}	0.930(3)	2.677(2)	3.606(3)	177(1)
C1–H1C···O1^{ii}	0.960(3)	2.803(2)	3.726(4)	161(2)
C15–H15A···N1^{iii}	0.970(3)	2.872(2)	3.597(4)	132(2)
H8–C_g1^{iv}	0.930(3)	3.217(6)	3.230(3)	132(1)

Symmetry code: (i) -x+1, -y+2, -z+1 (ii) x, + y-1, +z (iii) -x, +y+1/2, -z+1/2 (iv) -x+2, +y+1/2, -z-1/2

4. Conclusion

In the compound **3**, diethyl-dithiocarbamic acid is substituted at C- 4. The methyl group is substituted at C-6 position to the coumarin moiety.



In the molecule, the coumarin moiety is planar with dihedral angle 1.28(7) ˚ between the least-squares plane of the phenyl and pyrone rings. Bond lengths and bond angles in the coumarin moiety are typical for coumarin derivatives. The coumarin molecule is effectively flat with a deviation between the components in 6-membered rings of 0.84˚. The C3-C4 bond is conjugated to the carbonyl group, giving it a Michael acceptor function, characteristic of certain chemo preventive agents. The supramolecular structures of **3** was investigated in terms of C-H..O, C-H...S, C-H…N intermolecular interactions. In **3**, the C-H…O and C-H…S interactions generate dimers corresponding graph set motif $R^2_2(8)$ and $R^2_2(22)$ respectively whereas C-H…N interactions forms chain of molecules. In addition, the supramolecular cohesion is further strengthened by π-π stacking and C-H…π interactions in the compound.

The above compound possesses diverse pharmacological properties and biological activities. A single crystal x-ray diffraction analysis was carried out to establish the crystal structure and to understand the self-aggregation in terms of possible intermolecular interactions.

Data deposition

Crystallographic data for the structure reported here has been deposited with the Cambridge Data Centre. The deposition number is CCDC **877888.**

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Disclosure Statement

No potential conflict of interest was reported by the author

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