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3-Acetyl-7-(diethylamino)coumarin

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The title compound, $C_{15}H_{17}NO_3$, is nearly planar with a dihedral angle of 1.55 (10)° between the lactone and benzene rings. The molecules form chains through weak C—H···O hydrogen bonds and the chains are dimerized by type-II carbonyl–carbonyl interactions.

Comment

Coumarins are an important classe of molecules because of their applications in synthetic chemistry, medicinal chemistry, and photochemistry. Our group is interested in the synthesis and utility of novel Schiff base ligands (Hamaker & Halbach, 2006). In the course of our studies, we have prepared the title compound, (I), and determined its crystal structure.

(I)
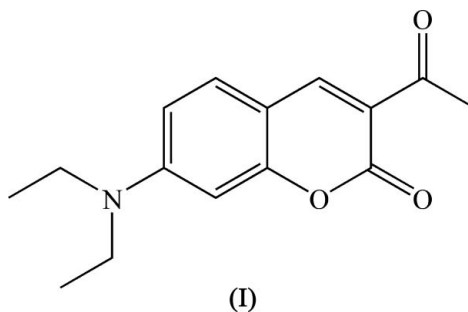
Compound (I) (Fig. 1) is essentially planar, with a dihedral angle between the lactone and benzene rings of 1.55 (10)°. The maximum deviation from planarity of the atoms in the benzene and lactone skeleton (C1–C9/O1) is 0.0271 (15) Å for atom C3. The plane of the acetyl group makes an angle with the C1–C9/O1 plane of 4.0 (2)°, which is smaller than that of related 7-acetylcoumarin derivatives (Kokila et al., 1996; Han et al., 2005). The C7/N15/C16/C18 group is essentially planar, with an r.m.s. deviation of 0.0204 Å. Also, the C7—N15 bond
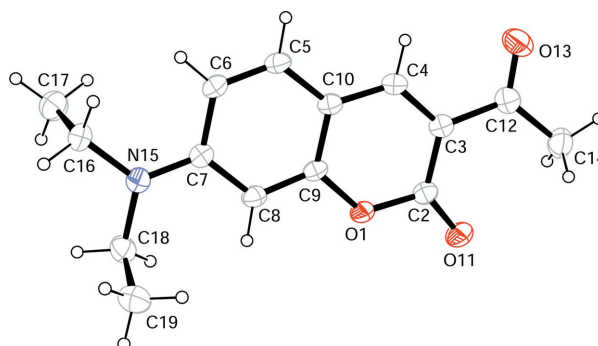

Figure 1
View of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids.
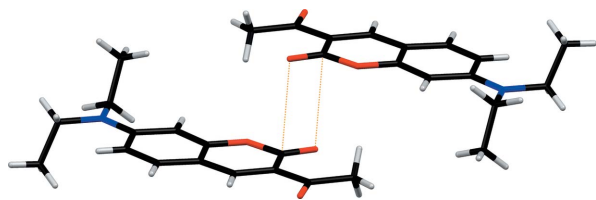
Figure 2
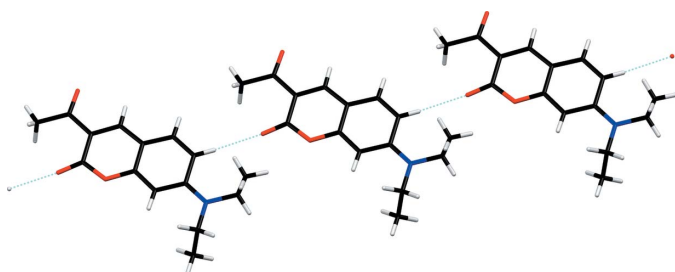View of a dimer of (I), showing the type-II carbonyl–carbonyl (orange dashed lines) interactions.

Figure 3
View of the C—H···O hydrogen bonding (cyan dashed lines) between the molecules.
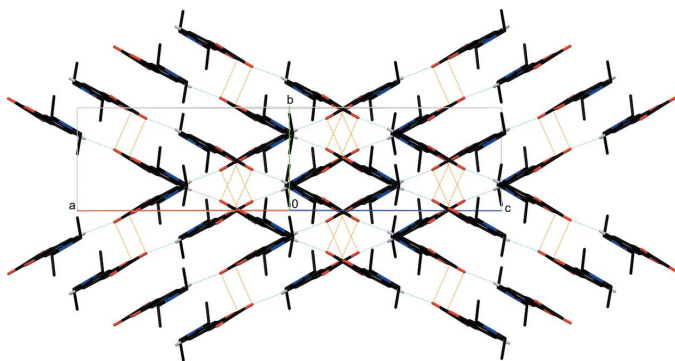

Figure 4
View of the intersecting double chains, viewed along the *ac* diagonal. C—H···O hydrogen bonds are shown in cyan and carbonyl–carbonyl interactions are shown in orange. H atoms not involved in hydrogen bonding have been omitted for clarity.

is significantly shorter than the C16—N15 and C18—N15 bonds (Table 1), indicating a donation of electrons from the N atom into the aromatic ring.

The molecules dimerize (Fig. 2) *via* a type-II carbonyl–carbonyl interaction (Allen *et al.*, 1998), with C2···O11^i and O11···C2^i distances of 3.139 (3) Å [symmetry code: (i) $\frac{1}{2} - x$, $-\frac{1}{2} - y, 1 - z$]. The molecules are linked together into chains in the crystal structure by weak C—H···O hydrogen bonds (Table 2 and Fig. 3). These double chains form a criss-cross network in the crystal structure when viewed along the *ac* diagonal (Fig. 4).

Experimental

Compound (I) was prepared by a previously described procedure (Aktoudianakis & Dicks, 2006). Single crystals were grown by slow evaporation of an ethanol solution.

Crystal data

$C_{15}H_{17}NO_3$	$Z = 8$
$M_r = 259.3$	$D_x = 1.266$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 17.269$ (2) Å	$\mu = 0.09$ mm^{-1}
$b = 7.5203$ (8) Å	$T = 297$ (2) K
$c = 22.0868$ (10) Å	Prism, red
$\beta = 108.524$ (7)°	$0.50 \times 0.50 \times 0.27$ mm
$V = 2719.8$ (5) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	1984 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$R_{int} = 0.018$
Absorption correction: none	$\theta_{max} = 27.5°$
3217 measured reflections	3 standard reflections
3118 independent reflections	frequency: 120 min
	intensity decay: 3%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1085P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$+ 0.3073P]$
$wR(F^2) = 0.199$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.18$	$(\Delta/\sigma)_{max} < 0.001$
3118 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
173 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C7—N15	1.365 (2)	C18—N15	1.461 (3)
C16—N15	1.466 (3)		
C18—N15—C16	116.05 (17)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O11^i	0.93	2.40	3.312 (2)	168

Symmetry code: (i) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

The H atoms were treated as riding atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = $1.2U_{eq}$(C) for the aromatic and methylene H atoms and U_{iso}(H) = $1.5U_{eq}$(C) for the methyl H atoms.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Bruno *et al.*, 2002) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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