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7-Cinnamoyloxy-4-methylcoumarin

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Key indicators

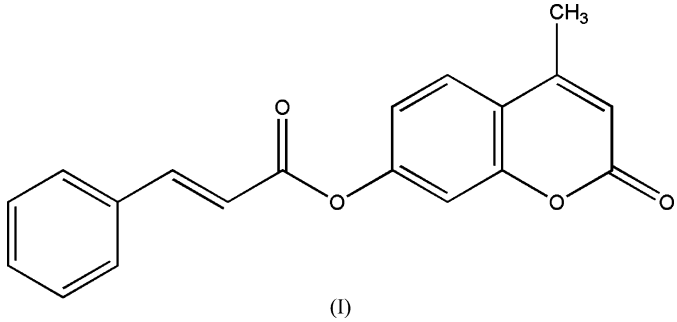
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.130
Data-to-parameter ratio = 12.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound [systematic name: 4-methyl-7-(3-phenylpropenoyl)oxy-2*H*-1-benzopyran-2-one], $C_{19}H_{14}O_4$, the coumarin moiety is almost perpendicular to the phenyl ring. There is one weak intramolecular C—H···O interaction.

Comment

Coumarins constitute an important class of natural products and synthetic compounds which exhibit a wide variety of pharmacological activities, such as anti-HIV activity (Xie *et al.*, 2001), antibacterial activity (Tanitame *et al.*, 2004) and the inhibition of acetylcholinesterase (AChE) (Brühlmann *et al.*, 2001). We present here the crystal structure of the title coumarin derivative, (I).



(I)

The C12═C13 bond is in the *trans* configuration. The coumarin moiety and the phenyl ring enclose a dihedral angle of 87.37 (6)°. The geometric parameters for (I) are normal. The crystal structure exhibits one weak intramolecular C—H···O interaction.

Experimental

The title compound was prepared as follows. To a solution containing 4-methyl-7-hydroxycoumarin (1.76 g, 10 mmol) and anhydrous

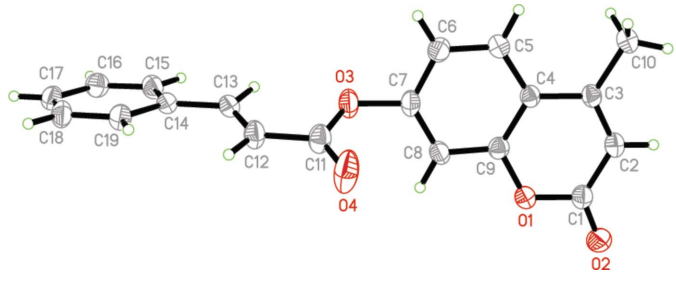


Figure 1
A view of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

pyridine (10 ml), a solution of cinnamyl chloride (1.75 g, 10 mmol) and anhydrous acetone (10 ml) was slowly added at 278–283 K with stirring for 30 min. The reaction mixture was stirred continuously for 24 h at room temperature (298–300 K) and then poured into ice–water (200 ml). The solid obtained was filtered off, washed with water and dried at room temperature. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 426–427 K).

Crystal data

$C_{19}H_{14}O_4$
M_r = 306.30
Triclinic, $P\overline{1}$
a = 7.349 (2) Å
b = 10.420 (3) Å
c = 10.658 (3) Å
α = 79.076 (5)°
β = 71.784 (4)°
γ = 78.503 (5)°
V = 752.6 (4) Å^3
Z = 2
D_x = 1.352 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Prism, colourless
0.48 × 0.45 × 0.40 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.956, T_{max} = 0.963
3995 measured reflections
2636 independent reflections
1596 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.130
S = 0.99
2636 reflections
210 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997*a*)
Extinction coefficient: 0.090 (7)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O3	0.93	2.38	2.731 (3)	102

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms, and C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for all other H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Brühlmann, C., Ooms, F., Carrupt, P.-A., Testa, B., Catto, M., Leonetti, F., Altomare, C. & Carotti, A. (2001). *J. Med. Chem.* **44**, 3195–3198.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen,Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Versions 4.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tanitame, A., Oyamada, Y., Ofuji, K., Fujimoto, M., Iwai, N., Hiyama, Y., Suzuki, K., Ito, H., Terauchi, H., Kawasaki, M., Nagai, K., Wachi, M. & Yamagishi, J. (2004). *J. Med. Chem.* **47**, 3693–3696.
Xie, L., Takeuchi, Y., Cosentino, L. M., McPhail, A. T. & Lee, K. H. (2001). *J. Med. Chem.* **44**, 664–671.