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#### Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.045  
 $wR$  factor = 0.118  
Data-to-parameter ratio = 10.0

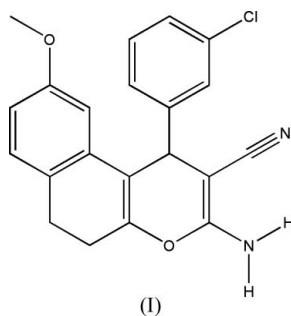
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 3-Amino-1-(2-chlorophenyl)-9-methoxy-5,6-dihydro-1*H*-benzo[*f*]chromene-2-carbonitrile

The title compound,  $\text{C}_{21}\text{H}_{17}\text{Cl}_1\text{N}_2\text{O}_2$ , was synthesized by the reaction of 7-methoxy-2-tetralone, 2-chlorobenzaldehyde and malononitrile in the presence of triethylbenzylammonium chloride in an aqueous medium. X-ray analysis reveals that the pyran ring and the fused six-membered ring adopt boat and half-chair conformations, respectively.

#### Comment

4*H*-Chromene compounds with amine and cyano groups are the synthons of some special natural products (Hatakeyama *et al.*, 1998; O'Callaghan & McMurry, 1995). We have recently developed new and environmentally friendly methodologies for the preparation of fine chemicals (Shi *et al.*, 2003). We have now synthesized the title compound, (I), in an aqueous medium and we report here its synthesis and crystal structure.



The molecular structure of (I) is shown in Fig. 1. The pyran ring can be regarded as having a boat conformation, for atoms O1 and C3 deviate from the C1/C2/C4/C13 plane in the same direction by 0.166 (3) and 0.279 (4) Å, respectively. The fused six-membered ring (C4/C5/C10–C13) adopts a half-chair conformation, in which atoms C11 and C12 are out of the C10/C5/C4/C13 plane by 0.260 (5) and 0.320 (5) Å in opposite directions, respectively.

The crystal packing of (I) is stabilized not only by the intermolecular hydrogen bonds between the amine group and atom N2 of the cyano group, but also by  $\text{C}-\text{H}\cdots\pi$  interactions involving the (C15–C20) benzene ring (centroid Cg1) (Table 1).

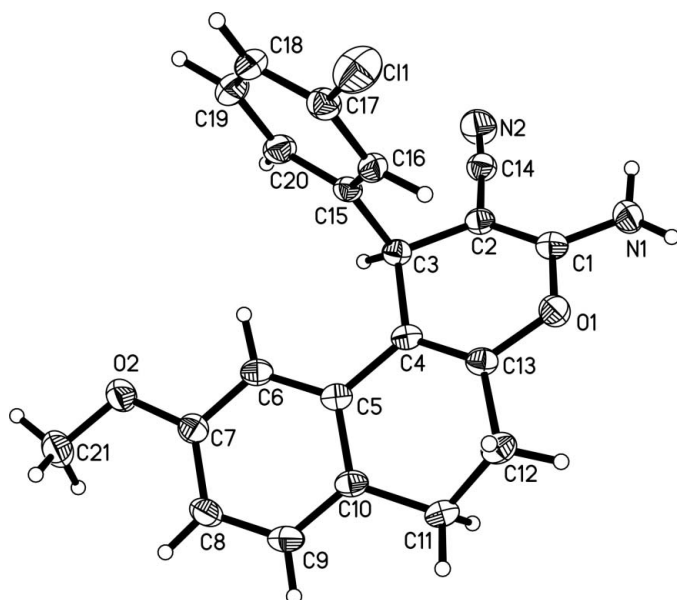
#### Experimental

The title compound was prepared by the reaction of 2-chlorobenzaldehyde (0.28 g, 2 mmol), 7-methoxy-2-tetralone (0.35 g, 2 mmol) and malononitrile (0.13 g, 2 mmol) in the presence of triethylbenzylammonium chloride (0.2 g) in water (10 ml) at 298 K for 25 h (yield 83%). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

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**Figure 1**  
The structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme.

#### Crystal data

$C_{21}H_{17}ClN_2O_2$   
 $M_r = 364.82$   
 Triclinic,  $P\bar{1}$   
 $a = 7.105$  (3) Å  
 $b = 9.762$  (3) Å  
 $c = 13.290$  (5) Å  
 $\alpha = 100.018$  (5)°  
 $\beta = 99.912$  (5)°  
 $\gamma = 100.614$  (4)°  
 $V = 872.0$  (5) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.389$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1477 reflections  
 $\theta = 2.4$ – $24.6$ °  
 $\mu = 0.24$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Prism, colourless  
 $0.31 \times 0.23 \times 0.15$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.930$ ,  $T_{\max} = 0.965$   
 4542 measured reflections

3036 independent reflections  
 2015 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$   
 $\theta_{\text{max}} = 25.0$ °  
 $h = -7 \rightarrow 8$   
 $k = -11 \rightarrow 10$   
 $l = -15 \rightarrow 12$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.118$   
 $S = 1.03$   
 3036 reflections  
 303 parameters

All H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0567P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.33$  e Å<sup>-3</sup>

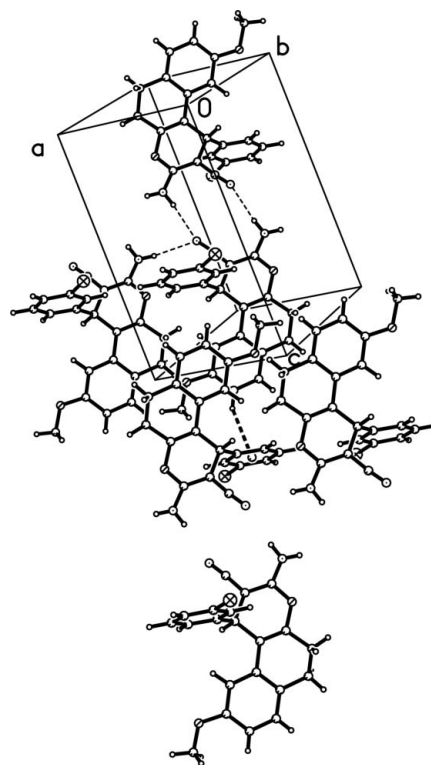
**Table 1**

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C15–C20 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots N2^i$	0.85 (3)	2.60 (3)	3.430 (4)	165 (3)
$N1-H2\cdots N2^{ii}$	0.86 (3)	2.24 (3)	3.088 (4)	172 (3)
$C8-H5\cdots Cg1^{iii}$	0.93 (2)	3.19 (4)	3.897 (2)	137 (2)

Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $-x + 1, -y, -z + 2$ .



**Figure 2**

The molecular packing in the crystal structure of (I). Intermolecular hydrogen bonds are shown as dashed lines.

H atoms were found in a difference Fourier map and their displacement parameters were refined freely.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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