

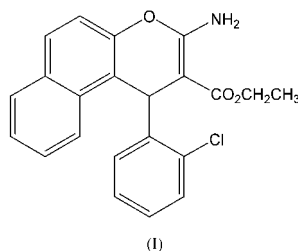
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## Key indicators

Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.033  
 $wR$  factor = 0.086  
Data-to-parameter ratio = 9.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2-Amino-4-(2-chlorophenyl)-3-ethoxy-  
carbonyl-4*H*-benzo[*f*]chromeneThe title compound,  $\text{C}_{22}\text{H}_{18}\text{ClNO}_3$ , was synthesized by the  
reaction of 2-naphthol with 2-chlorobenzaldehyde and ethyl  
cyanoacetate. X-ray analysis reveals that the pyran ring adopts  
a boat conformation.

## Comment

*4H*-chromene is a construction unit of some natural products.  
*4H*-chromenes with amino and cyano groups are also the  
synthon of some special natural products (Hatokeyama *et al.*,  
1998; O'Callaghan & McMurry, 1995). We have already  
reported the synthesis of some *4H*-chromene derivatives (Shi  
*et al.*, 2002; Zhuang *et al.*, 2002). We report here the X-ray  
crystal structure of the title compound, (I).The pyran ring adopt a boat conformation (Fig. 1); atoms  
C1, C2, C4 and C5 are coplanar, with atoms O1 and C3  
deviating from the plane by 0.236 (2) and 0.350 (2) Å,  
respectively. The bond lengths and angles in (I) show normal  
values (Table 1). An intramolecular hydrogen bond is formed  
between the amino group and atom O3 of the carbonyl group.  
The molecules are linked by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds,  
forming polymers (Fig. 2 and Table 2).

## Experimental

The title compound, (I), was prepared by the reaction of 2-naphthol  
with 2-chlorobenzaldehyde and ethyl cyanoacetate in ethanol in the  
presence of piperidine as catalyst. Single crystals (m.p. 448–450 K)  
suitable for X-ray diffraction were obtained by slow evaporation of  
an *N,N*-dimethylformamide–water solution.

## Crystal data

 $\text{C}_{22}\text{H}_{18}\text{ClNO}_3$   
 $M_r = 379.82$   
Monoclinic,  $Cc$   
 $a = 13.491$  (4) Å  
 $b = 13.375$  (4) Å  
 $c = 9.903$  (3) Å  
 $\beta = 93.51$  (2)°  
 $V = 1783.6$  (9) Å<sup>3</sup>  
 $Z = 4$  $D_x = 1.414$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 27  
reflections  
 $\theta = 2.9$ – $14.4$ °  
 $\mu = 0.24$  mm<sup>-1</sup>  
 $T = 292$  (2) K  
Block, colorless  
 $0.58 \times 0.50 \times 0.24$  mm

## Data collection

Siemens P4 diffractometer  
 $\omega$  scans  
 Absorption correction:  $\psi$  scan  
 (XSCANS; Siemens, 1994)  
 $T_{\min} = 0.851$ ,  $T_{\max} = 0.944$   
 3465 measured reflections  
 2449 independent reflections  
 2269 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = -16 \rightarrow 11$   
 $k = -11 \rightarrow 15$   
 $l = -11 \rightarrow 11$   
 3 standard reflections  
 every 97 reflections  
 intensity decay: 3.4%

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.086$   
 $S = 1.11$   
 2449 reflections  
 253 parameters  
 H atoms treated by a mixture of  
 independent and constrained  
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.0762P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.23 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$   
 Absolute structure: Flack (1983),  
 876 Friedel pairs  
 Flack parameter =  $-0.11(7)$

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1—C1	1.363 (3)	C1—C2	1.366 (3)
O1—C5	1.400 (3)	C2—C3	1.521 (3)
N—C1	1.340 (3)	C3—C4	1.534 (3)
C1—O1—C5	117.06 (19)	C1—C2—C14	119.2 (2)
N—C1—O1	110.0 (2)	C1—C2—C3	120.0 (2)
N—C1—C2	128.0 (3)	C5—O1—C1—N	158.8 (2)
C5—O1—C1—N	158.8 (2)	N—C1—C2—C14	-5.1 (4)
N—C1—C2—C14	-5.1 (4)	C1—C2—C3—C4	29.0 (3)
C1—C2—C3—C17	-93.5 (3)	C1—O1—C5—C4	24.8 (4)

Table 2

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N—H1A $\cdots$ O3	0.89 (3)	2.08 (3)	2.709 (4)	127 (2)
N—H1B $\cdots$ O3 <sup>i</sup>	0.84 (3)	2.19 (3)	3.029 (3)	172 (3)

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

The amino H atoms H1A and H1B were refined isotropically. Positions of the other H atoms were fixed geometrically and distances to H atoms were set by the program. ( $C-H$  0.93–0.98  $\text{\AA}$ ;  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ ).

Data collection: XSCANS (Siemens, 1994); cell refinement: XSCANS; data reduction: SHELXTL (Sheldrick, 1997); program(s) used to solve structure: SHELXTL; program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

We thank the Foundation of the Surpassing Project of Jiangsu Province for financial support.

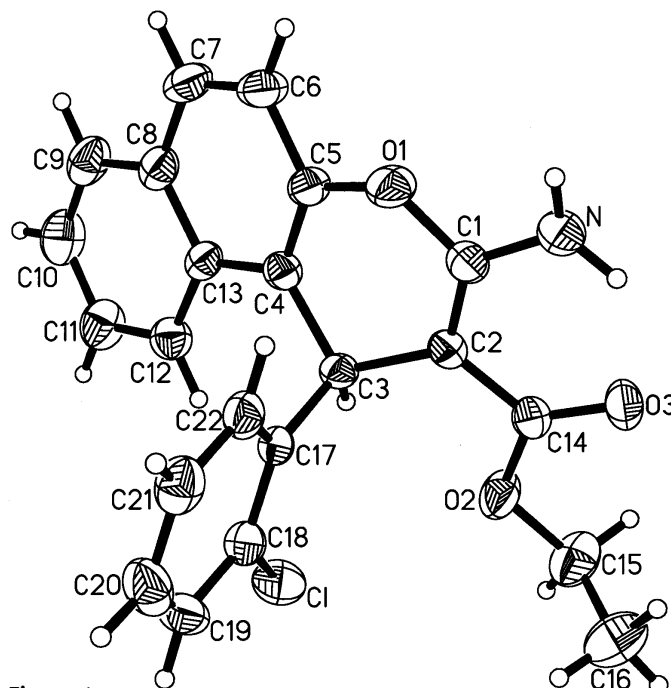


Figure 1

The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

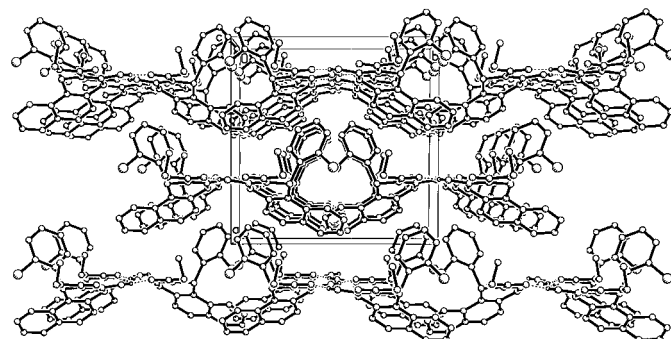


Figure 2

A molecular packing diagram of the crystal structure of (I).

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