Cell refinement: *KM-4 Software* (Kuma, 1997). Data reduction: *KM-4 Software*. Program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990*a*). Program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997). Molecular graphics: *SHELXTL* (Sheldrick, 1990*b*). Software used to prepare material for publication: *SHELXL97*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: KA1282). Services for accessing these data are described at the back of the journal.

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2,3-Dihydrodioxin[2,3-*b*]acridin-11(6*H*)-one

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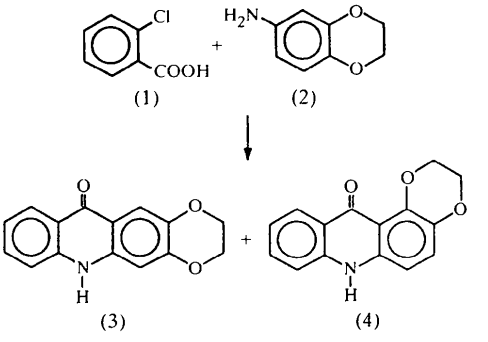
Abstract

The title compound, $C_{15}H_{11}NO_3$, belongs to a series of new potential antiviral agents against the herpes virus containing a fused ring system. The acridinone skeleton adopts a boat conformation, with greater folding at the junction with the dioxane ring. This ring is twisted with an approximate twofold axis bisecting the two C—C bonds.

Comment

This work has been undertaken in the context of our studies on acridine derivatives with potential pharmacological properties. Acridines are a well known group of antibacterial, antitumour and antifungal drugs (Babu *et al.*, 1986; Miyahara *et al.*, 1982; Crémieux *et al.*, 1994; Karolak-Wojciechowska *et al.*, 1996). Recently our attention has been focused on dioxanoacridinones obtained by condensing 2-chlorocarboxylic acid (1) and 1,4-benzodioxan-6-amine (2) (see scheme). According to



the Ullmann's reaction, two isomers can be obtained [(3) and (4)]. These dioxanoacridinones, (3) and (4), are under investigation as potential antiviral agents against the herpes virus (Mucsi *et al.*, 1997). With the aim of comparing the biological activity of the isomers with their structures, the title compound (3) has been the subject of an X-ray investigation. The choice of molecule (3) rather than (4) was based on crystal quality. The molecule of (3) is presented in Fig. 1 and therefore the structures of both isomers are confirmed.

Besides the confirmation of the chemical structure, some interesting structural observations in the geometry of the molecule of (3) can be made. The basic acridi-

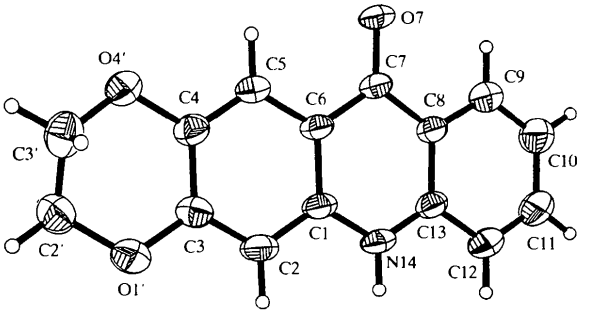


Fig. 1. Molecular structure of (3) showing 50% probability displacement ellipsoids.

none skeleton (with conjugated bonds) adopts a boat conformation [the boat is more folded at the junction with the fourth ring, dioxane]. This is clearly demonstrated by the values of the dihedral angles formed by the following planes: *A*1 (defined by the atoms C8, C9, C10, C11, C12 and C13), *A*2 (C1, N14, C13, C8, C7 and C6) and *A*3 (C1, C2, C3, C4, C5 and C6) where *A*1/*A*2 = 1.07 (4)°, *A*2/*A*3 = 2.41 (4)° and *A*1/*A*3 = 3.3 (1)°. The conformation of the acridinone moiety fits well with those of several acridinone derivatives in the Cambridge Structural Database (Allen & Kennard, 1993). The dioxane contains two C_{sp^2} atoms (C3 and C4). Consequently these atoms and both O atoms (O1′ and O4′) are coplanar. The two remaining atoms C2′ and C3′ are out of the plane defined by the atoms C3, C4, O4′ and O1′, by 0.376 (2) Å and −0.282 (2) Å, respectively. Therefore the dioxane ring conformation can be described as twisted with an approximate twofold symmetry axis bisecting the C3—C4 and C2′—C3′ bonds. The relevant torsion angles are given in Table 1. This ring is folded inside the acridone boat and the mean plane of all six dioxane ring atoms (*A*4) is inclined to the plane *A*2 by 4.96 (4)°. In the crystal, the molecules of (3) are packed in columns down the *x* axis with a distance between molecules of about 2.6 Å. Columns are linked by an intermolecular hydrogen bond, N14—H14*A*···O7^{i} [N14···O7^{i} = 2.8039 (16) Å; symmetry operation: (i) *x*, $\frac{1}{2} - y$, $\frac{1}{2} + z$]. All bond distances and angles have typical values.

Experimental

Compound (3) was obtained from 2-chlorocarboxylic acid and 1,4-benzodioxan-6-amine (Galy *et al.*, 1996) and then crystallized from ethanol.

Crystal data

$C_{15}H_{11}NO_3$
M_r = 253.25
Monoclinic
$P2_1/c$
a = 5.161 (1) Å
b = 17.694 (4) Å
c = 13.155 (3) Å
β = 96.64 (3)°
V = 1193.2 (4) Å^3
Z = 4
D_x = 1.410 Mg m^{-3}
D_m not measured
Cu $K\alpha$ radiation
λ = 1.54178 Å
Cell parameters from 25 reflections
θ = 15–45°
μ = 0.818 mm^{-1}
T = 293 K
Block cut from plate
0.4 × 0.2 × 0.2 mm
Colourless

Data collection

Kuma KM-4 diffractometer
ω–2θ scans
Absorption correction: none
2320 measured reflections
2224 independent reflections
2039 reflections with $I > 2\sigma(I)$
R_{int} = 0.0213
θ_{max} = 80.74°
$h = -6 \rightarrow 6$
$k = 0 \rightarrow 22$
$l = -16 \rightarrow 0$
2 standard reflections
every 100 reflections
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.112
S = 1.11
2224 reflections
173 parameters
H atoms riding
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.2885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0060 (7)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters* (°)

C2′—O1′—C3—C4	17.6 (2)	C4—O4′—C3′—C2′	−45.68 (18)
C3—O1′—C2′—C3′	−47.19 (19)	O1′—C2′—C3′—O4′	62.46 (18)
C3′—O4′—C4—C3	16.0 (2)	O1′—C3—C4—O4′	−0.8 (2)

H atoms were refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C/N).

Data collection: *KM*4 (Kuma Diffraction, 1992). Cell refinement: *KM*4. Data reduction: *DATARED* (Kuma Diffraction, 1992). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93. Molecular graphics: *XP* (Sheldrick, 1993). Software used to prepare material for publication: *SHELXL*93.

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