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# 11-(4-Fluorophenyl)-7,11-dihydrobenzo[*f*]furo-[3,4-*b*]quinolin-10(8*H*)-one

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The title compound, $C_{21}H_{14}FNO_2$, was synthesized by the reaction of 4-fluorobenzaldehyde, 2-naphthylamine and tetronic acid in water under microwave irradiation. The dihydropyridine ring adopts a flattened boat conformation. N—H···O hydrogen bonds link symmetry-related molecules into a chain along the *b* axis.

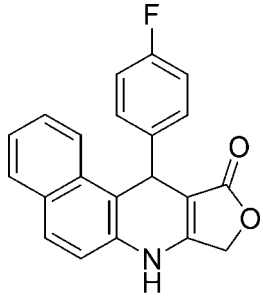
**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.006 Å
*R* factor = 0.049
*wR* factor = 0.136
Data-to-parameter ratio = 12.0

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

## Comment

Tetronic acid derivatives and their metabolites, of which vitamin C and penicillic acid are undoubtedly the most important, are widespread in nature (Neelakantan & Seshadri, 1959). Natural 4-ylidenetetronic acid derivatives known as pulvinic acids have been found as pigments in lichens and higher fungi (Weinstock *et al.*, 1979). Tetronic acid derivatives are interesting because of their antibiotic, antitumour, anti-coagulant, anti-epileptic, antifungal and anti-inflammatory properties (Foden & McCormick, 1975). We report here the crystal structure of the title compound, (I).




(I)

The dihydropyridine ring adopts a flattened boat conformation, with atoms N1 and C5 deviating from the C2/C3/C6/C7 plane by 0.084 (5) and 0.128 (5) Å, respectively (Fig. 1). The dihedral angle between the C2/C3/C6/C7 and the C16–C21 planes is 81.1 (1)°. The naphthalene and the furanone ring systems form dihedral angles of 4.6 (2) and 6.3 (2)°, respectively, with the C2/C3/C6/C7 plane. The crystal structure shows that the molecules are connected *via* N—H···O hydrogen bonds (Table 1), forming a chain along the *b* axis.

## Experimental

Compound (I) was prepared by the reaction of 4-fluorobenzaldehyde (1 mmol), 2-naphthylamine (1 mmol) and tetronic acid (1 mmol) in water (2 ml) under microwave irradiation for 3 min. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 85%; m.p. 573 K).

*Crystal data*

$C_{21}H_{14}FNO_2$
$M_r$ = 331.33
Monoclinic, $C2/c$
$a$ = 21.010 (7) Å
$b$ = 11.388 (4) Å
$c$ = 15.123 (5) Å
$\beta$ = 121.380 (5)°
$V$ = 3089.1 (18) Å$^3$
$Z$ = 8
$D_x$ = 1.425 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 298 (2) K
Block, yellow
0.23 × 0.18 × 0.16 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.977, $T_{max}$ = 0.984
7962 measured reflections
2723 independent reflections
1227 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055
$\theta_{max}$ = 25.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.136
$S$ = 0.99
2723 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 3.6851P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.86 | 2.20 | 2.885 (4) | 137 |

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were positioned geometrically and treated as riding, with C—H distances of 0.93–0.98 Å, N—H = 0.86 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C,N).

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*.

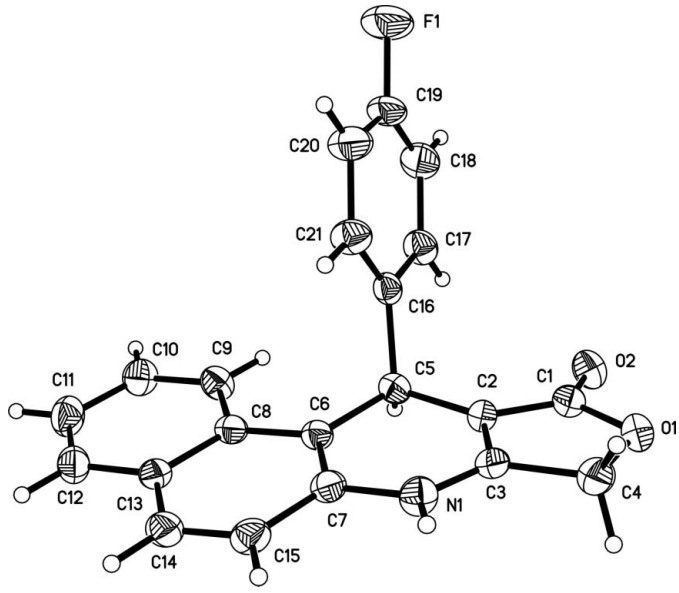



**Figure 1**
The structure of (I), showing 30% probability displacement ellipsoids.

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