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2′-[2-(4-Fluorophenyl)chroman-4-ylidene]-isonicotinohydrazide

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Key indicators

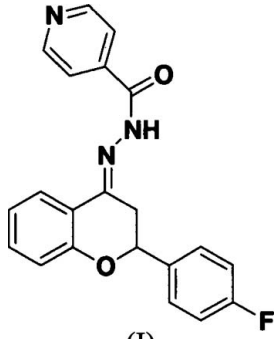
Single-crystal X-ray study
T = 208 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.128
Data-to-parameter ratio = 12.0

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

In the title compound, $C_{21}H_{16}FN_3O_2$, the pyridine ring is nearly coplanar with the plane of the fused bicyclic ring system [dihedral angle = 4.1 (2)°], while the 4-fluorophenyl ring forms a dihedral angle of 67.7 (3)° with the fused bicyclic ring system.

Comment

Flavonoids are polyphenolic compounds that are categorized according to their chemical structure into flavonols, flavones, flavanones, isoflavones, catechins, anthocyanidins and chalcones. Over 4 000 flavonoids have been identified, many of which occur in fruit, vegetables and beverages. Flavonoids have attracted considerable interest recently because of their potential beneficial effects for human health. They have been reported to have antiviral, anti-allergic, antiplatelet, anti-inflammatory, and anti-oxidant activities. It has also been demonstrated recently that flavanone and its derivatives have potential bioactivities against cancer (Senderowicz, 1999; Brueggemeier *et al.*, 2001; Bauvois *et al.*, 2003). To investigate the anticancer activity of such compounds, we have synthesized a library of new flavanone derivatives, by a microwave-assisted methodology, including the title compound, (I).



(I)

All bond lengths and angles in (I) (Fig. 1) are within normal ranges (Allen *et al.*, 1987). The pyridine ring is nearly coplanar with the fused bicyclic ring system [dihedral angle = 4.1 (2)°], while the 4-fluorophenyl ring makes a dihedral angle of 67.7 (3)° with the central ring system. In the crystal structure, molecules are linked into dimers by N2—H2···O2^{i} hydrogen bonds [H2···O2^{i} = 2.09, N2···O2^{i} = 2.942 (2) Å, N2—H2···O2^{i} = 165°; symmetry code: (i) 2 − *x*, −1 − *y*, 1 − *z*].

Experimental

For the preparation of (I), 3-(4-fluorophenyl)-1-(2-hydroxyphenyl)propenone (60.5 mg, 0.25 mmol) and isonicotinohydrazide (35 mg, 0.25 mmol) were dissolved in 2-propanol (1 ml). The solution was

heated for 2 h at 393 K by microwave irradiation. After cooling to room temperature, the resulting precipitate was collected by filtration and dried, yielding (I) as a yellow solid (20.0 mg, 21%). This was crystallized from an ethanol solution to afford crystals suitable for X-ray analysis.

Crystal data

$C_{21}H_{16}FN_3O_2$
M_r = 361.37
Monoclinic, $P2_1/c$
a = 11.654 (5) Å
b = 5.471 (2) Å
c = 26.609 (10) Å
β = 102.416 (6)°
V = 1656.9 (11) Å^3
Z = 4
D_x = 1.449 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 208 (2) K
Plate, yellow
0.20 × 0.20 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.993
9130 measured reflections
2933 independent reflections
2219 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.128
S = 1.05
2933 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.1714P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

All H atoms were included in the riding-model approximmation, with C—H = 0.94–0.99 Å, N—H = 0.87 Å and U_{iso}(H) = 1.2U_{eq}(N,C).

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-32* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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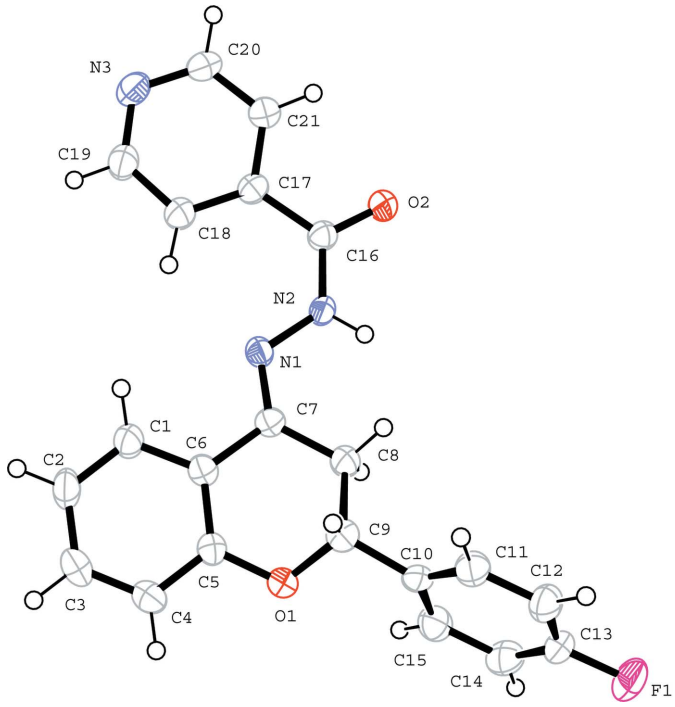

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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