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5-(4-Fluorophenyl)-2,6-dioxo-2,3,6,7,-8,9-hexahydro-1*H*,5*H*-imidazo[1,2-*a*]-quinoline-4-carbonitrile

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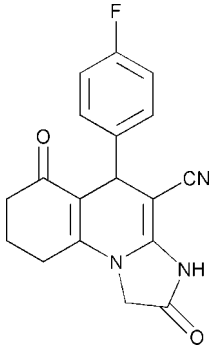
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.112; data-to-parameter ratio = 12.3.

In the molecule of the title compound, $C_{18}H_{14}FN_3O_2$, the imidazole and dihydropyridine rings are nearly coplanar with a dihedral angle of 2.46 (3)°, while the cyclohexene ring has an envelope conformation. The benzene ring is oriented with respect to the coplanar ring system at a dihedral angle of 81.45 (2)°. In the crystal structure, intermolecular N—H···N hydrogen bonds link the molecules into dimers.

Related literature

For related literature, see: Stout & Meyers (1982); Gueiffier *et al.* (1996); Elhakmaoui *et al.* (1994). For general background, see: Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{14}FN_3O_2$
M_r = 323.32
Monoclinic, $P2_1/c$
a = 10.781 (3) Å
b = 14.937 (4) Å
c = 9.839 (3) Å
β = 106.270 (5)°
V = 1521.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.36 × 0.33 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.981
7885 measured reflections
2678 independent reflections
1368 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.112
S = 1.00
2678 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N3^{i}	0.86	2.15	3.006 (4)	173

Symmetry code: (i) $-x+2, -y, -z$.

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2320).

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supplementary materials

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5-(4-Fluorophenyl)-2,6-dioxo-2,3,6,7,8,9-hexahydro-1*H*,5*H*-imidazo[1,2-*a*]quinoline-4-carbonitrile

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Comment

1,4-Dihydropyridines (1,4-DHPs) are well known compounds because of their pharmacological profiles as calcium channel modulators (Stout & Meyers, 1982). With a 1,4-DHPs parent nucleus, imidazo[1,2-*a*]quinoline belongs to a class of compounds which are special not only because of their interesting chemical and physical properties, but also due to their immense utility in the pharmaceutical industries. The discovery of imidazo[1,2-*a*]quinoline including imidazo[1,2-*a*]- pyridine moiety, as new potential pharmacological molecules, may be of great significance. It is well established that the chemical modifications on the imidazo[1,2-*a*]pyridine skeletons may bring remarkable changes of biological activity (Gueiffier *et al.*, 1996; Elhakmaoui *et al.*, 1994). We report herein the crystal structure of the title compound, (I).

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

Ring A (C1—C6) is not planar, having total puckering amplitude, Q_T, of 0.488 (3) Å, [φ = −64.74 (3)°, θ = 117.65 (3)°] (Cremer & Pople, 1975), and adopts an envelope conformation with atom C3 displaced by −0.663 (3) Å from the plane of the other ring atoms. Rings B (N1/C1/C6—C9), C (N1/N2/C9—C11) and D (C13—C18) are, of course, planar and rings B and D are also nearly coplanar with a dihedral angle of 2.46 (3)°. Ring D is oriented with respect to the coplanar ring system at a dihedral angle of 81.45 (2)°.

In the crystal structure, the intermolecular N—H···N hydrogen bonds (Table 1) link the molecules into dimers (Fig. 2), in which they seem to be effective in the stabilization of the structure.

Experimental

The title compound, (I), was prepared by the reaction of 4-fluorobenzaldehyde (124 mg, 1 mmol), 2-(3-oxocyclohex-1-enylamino)acetic acid (169 mg, 1 mmol) with malononitrile (66 mg, 1 mmol) in solvent of ethylene glycol (2.0 ml) at 393 K under microwave irradiation (maximum power 200 W, initial power 100 W) for 5 min. Single crystals suitable for X-ray analysis were obtained from an ethanol solution (95%) by slow evaporation (yield; 284 mg, 88%, m.p. 559–560 K).

Refinement

H atoms were positioned geometrically with N—H = 0.86 Å (for NH) and C—H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

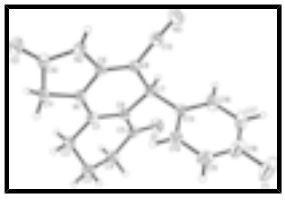

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

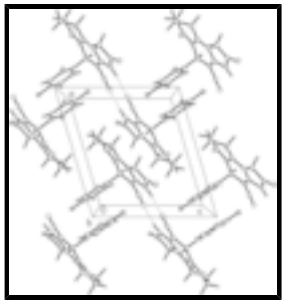

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

5-(4-Fluorophenyl)-2,6-dioxo-2,3,6,7,8,9-hexahydro-1H,5*H*- imidazo[1,2-*a*]quinoline-4-carbonitrile

Crystal data

$C_{18}H_{14}FN_3O_2$	F_{000} = 672
M_r = 323.32	D_x = 1.412 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 559-560 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.781 (3) Å	Cell parameters from 1113 reflections
b = 14.937 (4) Å	θ = 2.4–21.3º
c = 9.839 (3) Å	μ = 0.10 mm^{-1}
β = 106.270 (5)º	T = 298 (2) K
V = 1521.0 (7) Å^3	Block, colourless
Z = 4	0.36 × 0.33 × 0.19 mm

Data collection

Bruker CCD area-detector diffractometer	2678 independent reflections
Radiation source: fine-focus sealed tube	1368 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.964, T_{max} = 0.981	k = −17→17
7885 measured reflections	l = −11→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 0.3811P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
2678 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
217 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.9987 (2)	−0.14960 (16)	0.7379 (2)	0.1056 (8)
N1	0.6362 (2)	0.12725 (14)	0.1016 (2)	0.0360 (6)
N2	0.7956 (2)	0.13795 (15)	0.0009 (2)	0.0395 (6)
H2	0.8621	0.1239	−0.0266	0.047*
N3	0.9607 (3)	−0.08486 (18)	0.0697 (3)	0.0617 (8)
O1	0.48004 (19)	−0.12894 (13)	0.2715 (2)	0.0531 (6)
O2	0.7643 (2)	0.28153 (14)	−0.0880 (2)	0.0619 (6)
C1	0.5553 (2)	0.08620 (19)	0.1683 (3)	0.0339 (7)
C2	0.4489 (3)	0.14201 (18)	0.1931 (3)	0.0414 (8)
H2A	0.3764	0.1426	0.1084	0.050*
H2B	0.4787	0.2031	0.2137	0.050*
C3	0.4061 (3)	0.10459 (19)	0.3161 (3)	0.0489 (8)
H3A	0.4749	0.1121	0.4033	0.059*
H3B	0.3312	0.1374	0.3251	0.059*
C4	0.3728 (3)	0.00648 (19)	0.2935 (3)	0.0464 (8)
H4A	0.3567	−0.0176	0.3785	0.056*
H4B	0.2940	0.0004	0.2169	0.056*
C5	0.4778 (3)	−0.0473 (2)	0.2589 (3)	0.0385 (7)

C6	0.5737 (3)	−0.00083 (18)	0.2071 (3)	0.0328 (7)
C7	0.6892 (3)	−0.05532 (17)	0.1965 (3)	0.0334 (7)
H7	0.6569	−0.1104	0.1445	0.040*
C8	0.7650 (3)	−0.00414 (18)	0.1131 (3)	0.0346 (7)
C9	0.7373 (3)	0.08079 (18)	0.0738 (3)	0.0341 (7)
C10	0.7359 (3)	0.2201 (2)	−0.0233 (3)	0.0419 (8)
C11	0.6280 (3)	0.21783 (17)	0.0460 (3)	0.0425 (8)
H11A	0.6414	0.2618	0.1213	0.051*
H11B	0.5450	0.2286	−0.0223	0.051*
C12	0.8730 (3)	−0.04756 (19)	0.0866 (3)	0.0418 (8)
C13	0.7743 (3)	−0.08156 (19)	0.3424 (3)	0.0355 (7)
C14	0.8134 (3)	−0.0171 (2)	0.4468 (3)	0.0450 (8)
H14	0.7881	0.0421	0.4268	0.054*
C15	0.8894 (3)	−0.0398 (3)	0.5800 (3)	0.0555 (9)
H15	0.9154	0.0035	0.6503	0.067*
C16	0.9252 (3)	−0.1262 (3)	0.6059 (4)	0.0638 (10)
C17	0.8917 (3)	−0.1908 (3)	0.5061 (4)	0.0716 (11)
H17	0.9197	−0.2494	0.5265	0.086*
C18	0.8151 (3)	−0.1678 (2)	0.3734 (4)	0.0554 (9)
H18	0.7907	−0.2117	0.3039	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0817 (15)	0.149 (2)	0.0675 (14)	0.0011 (15)	−0.0098 (12)	0.0457 (15)
N1	0.0427 (15)	0.0250 (13)	0.0445 (14)	0.0032 (12)	0.0189 (12)	0.0039 (11)
N2	0.0443 (15)	0.0360 (15)	0.0431 (15)	0.0017 (12)	0.0200 (12)	0.0053 (12)
N3	0.066 (2)	0.0445 (17)	0.089 (2)	0.0114 (15)	0.0466 (17)	0.0115 (16)
O1	0.0565 (14)	0.0360 (13)	0.0746 (16)	−0.0037 (11)	0.0311 (12)	0.0067 (12)
O2	0.0741 (16)	0.0412 (14)	0.0792 (16)	−0.0040 (12)	0.0361 (13)	0.0171 (12)
C1	0.0312 (16)	0.0373 (19)	0.0341 (17)	−0.0034 (14)	0.0104 (14)	−0.0040 (14)
C2	0.0454 (19)	0.0345 (18)	0.0479 (18)	0.0059 (15)	0.0191 (15)	0.0012 (15)
C3	0.056 (2)	0.045 (2)	0.055 (2)	0.0035 (16)	0.0294 (17)	−0.0027 (16)
C4	0.0434 (19)	0.048 (2)	0.053 (2)	0.0015 (16)	0.0234 (16)	0.0006 (16)
C5	0.0411 (19)	0.0371 (19)	0.0381 (17)	−0.0010 (16)	0.0126 (14)	0.0020 (15)
C6	0.0383 (17)	0.0283 (17)	0.0341 (16)	−0.0029 (14)	0.0143 (13)	−0.0023 (14)
C7	0.0407 (17)	0.0215 (15)	0.0401 (17)	−0.0001 (13)	0.0148 (14)	0.0011 (13)
C8	0.0379 (17)	0.0302 (18)	0.0401 (17)	0.0022 (14)	0.0181 (14)	0.0029 (14)
C9	0.0386 (17)	0.0331 (18)	0.0338 (16)	−0.0011 (14)	0.0153 (14)	0.0002 (14)
C10	0.049 (2)	0.0305 (18)	0.0471 (19)	−0.0030 (16)	0.0150 (16)	0.0051 (15)
C11	0.056 (2)	0.0264 (17)	0.0498 (18)	0.0045 (15)	0.0221 (16)	0.0050 (14)
C12	0.051 (2)	0.0280 (17)	0.0518 (19)	−0.0019 (16)	0.0232 (16)	0.0047 (15)
C13	0.0349 (17)	0.0298 (17)	0.0450 (18)	0.0016 (14)	0.0165 (14)	0.0066 (15)
C14	0.0413 (19)	0.046 (2)	0.047 (2)	0.0040 (15)	0.0130 (16)	0.0029 (16)
C15	0.045 (2)	0.077 (3)	0.046 (2)	−0.0005 (19)	0.0137 (17)	−0.0024 (19)
C16	0.045 (2)	0.089 (3)	0.052 (2)	−0.002 (2)	0.0055 (18)	0.024 (2)
C17	0.069 (3)	0.053 (3)	0.082 (3)	0.011 (2)	0.004 (2)	0.031 (2)
C18	0.060 (2)	0.034 (2)	0.067 (2)	0.0042 (17)	0.0087 (19)	0.0070 (17)

Geometric parameters (Å, °)

F1—C16	1.363 (4)	C5—C6	1.451 (4)
N1—C1	1.374 (3)	C6—C7	1.516 (3)
N1—C9	1.383 (3)	C7—C8	1.517 (3)
N1—C11	1.453 (3)	C7—C13	1.522 (4)
N2—C9	1.375 (3)	C7—H7	0.9800
N2—C10	1.375 (3)	C8—C9	1.335 (3)
N2—H2	0.8600	C8—C12	1.420 (4)
N3—C12	1.149 (3)	C10—C11	1.504 (4)
O1—C5	1.225 (3)	C11—H11A	0.9700
O2—C10	1.204 (3)	C11—H11B	0.9700
C1—C6	1.354 (4)	C13—C18	1.368 (4)
C1—C2	1.492 (3)	C13—C14	1.384 (4)
C2—C3	1.518 (4)	C14—C15	1.379 (4)
C2—H2A	0.9700	C14—H14	0.9300
C2—H2B	0.9700	C15—C16	1.351 (5)
C3—C4	1.510 (4)	C15—H15	0.9300
C3—H3A	0.9700	C16—C17	1.352 (5)
C3—H3B	0.9700	C17—C18	1.378 (4)
C4—C5	1.502 (4)	C17—H17	0.9300
C4—H4A	0.9700	C18—H18	0.9300
C4—H4B	0.9700		
C1—N1—C9	120.8 (2)	C8—C7—H7	107.9
C1—N1—C11	128.0 (2)	C13—C7—H7	107.9
C9—N1—C11	111.2 (2)	C9—C8—C12	120.6 (3)
C9—N2—C10	112.6 (2)	C9—C8—C7	121.7 (2)
C9—N2—H2	123.7	C12—C8—C7	117.6 (2)
C10—N2—H2	123.7	C8—C9—N2	130.1 (3)
C6—C1—N1	120.1 (2)	C8—C9—N1	122.9 (2)
C6—C1—C2	123.3 (2)	N2—C9—N1	107.0 (2)
N1—C1—C2	116.7 (2)	O2—C10—N2	126.5 (3)
C1—C2—C3	110.1 (2)	O2—C10—C11	126.9 (3)
C1—C2—H2A	109.6	N2—C10—C11	106.6 (2)
C3—C2—H2A	109.6	N1—C11—C10	102.6 (2)
C1—C2—H2B	109.6	N1—C11—H11A	111.2
C3—C2—H2B	109.6	C10—C11—H11A	111.2
H2A—C2—H2B	108.1	N1—C11—H11B	111.2
C4—C3—C2	110.6 (2)	C10—C11—H11B	111.2
C4—C3—H3A	109.5	H11A—C11—H11B	109.2
C2—C3—H3A	109.5	N3—C12—C8	177.3 (3)
C4—C3—H3B	109.5	C18—C13—C14	118.5 (3)
C2—C3—H3B	109.5	C18—C13—C7	121.6 (3)
H3A—C3—H3B	108.1	C14—C13—C7	119.9 (2)
C5—C4—C3	112.9 (2)	C15—C14—C13	120.8 (3)
C5—C4—H4A	109.0	C15—C14—H14	119.6
C3—C4—H4A	109.0	C13—C14—H14	119.6
C5—C4—H4B	109.0	C16—C15—C14	118.4 (3)

C3—C4—H4B	109.0	C16—C15—H15	120.8
H4A—C4—H4B	107.8	C14—C15—H15	120.8
O1—C5—C6	121.1 (3)	C15—C16—C17	122.7 (3)
O1—C5—C4	120.3 (3)	C15—C16—F1	119.0 (4)
C6—C5—C4	118.7 (3)	C17—C16—F1	118.3 (4)
C1—C6—C5	119.8 (3)	C16—C17—C18	118.5 (3)
C1—C6—C7	123.7 (2)	C16—C17—H17	120.7
C5—C6—C7	116.6 (2)	C18—C17—H17	120.7
C6—C7—C8	110.1 (2)	C13—C18—C17	121.0 (3)
C6—C7—C13	111.3 (2)	C13—C18—H18	119.5
C8—C7—C13	111.5 (2)	C17—C18—H18	119.5
C6—C7—H7	107.9		
C9—N1—C1—C6	−0.3 (4)	C7—C8—C9—N1	−2.2 (4)
C11—N1—C1—C6	176.6 (3)	C10—N2—C9—C8	178.1 (3)
C9—N1—C1—C2	−179.8 (2)	C10—N2—C9—N1	−1.1 (3)
C11—N1—C1—C2	−3.0 (4)	C1—N1—C9—C8	−2.2 (4)
C6—C1—C2—C3	24.5 (4)	C11—N1—C9—C8	−179.6 (3)
N1—C1—C2—C3	−156.0 (2)	C1—N1—C9—N2	177.0 (2)
C1—C2—C3—C4	−53.2 (3)	C11—N1—C9—N2	−0.3 (3)
C2—C3—C4—C5	51.4 (3)	C9—N2—C10—O2	−177.6 (3)
C3—C4—C5—O1	162.2 (3)	C9—N2—C10—C11	2.0 (3)
C3—C4—C5—C6	−19.4 (4)	C1—N1—C11—C10	−175.7 (2)
N1—C1—C6—C5	−171.3 (2)	C9—N1—C11—C10	1.4 (3)
C2—C1—C6—C5	8.3 (4)	O2—C10—C11—N1	177.6 (3)
N1—C1—C6—C7	7.2 (4)	N2—C10—C11—N1	−2.0 (3)
C2—C1—C6—C7	−173.3 (2)	C9—C8—C12—N3	153 (7)
O1—C5—C6—C1	167.3 (3)	C7—C8—C12—N3	−23 (7)
C4—C5—C6—C1	−11.1 (4)	C6—C7—C13—C18	130.9 (3)
O1—C5—C6—C7	−11.2 (4)	C8—C7—C13—C18	−105.8 (3)
C4—C5—C6—C7	170.3 (2)	C6—C7—C13—C14	−49.9 (3)
C1—C6—C7—C8	−10.3 (4)	C8—C7—C13—C14	73.4 (3)
C5—C6—C7—C8	168.2 (2)	C18—C13—C14—C15	−1.4 (4)
C1—C6—C7—C13	113.9 (3)	C7—C13—C14—C15	179.4 (2)
C5—C6—C7—C13	−67.7 (3)	C13—C14—C15—C16	0.3 (4)
C6—C7—C8—C9	7.7 (4)	C14—C15—C16—C17	1.3 (5)
C13—C7—C8—C9	−116.4 (3)	C14—C15—C16—F1	−179.0 (2)
C6—C7—C8—C12	−176.8 (2)	C15—C16—C17—C18	−1.7 (5)
C13—C7—C8—C12	59.2 (3)	F1—C16—C17—C18	178.6 (3)
C12—C8—C9—N2	3.4 (5)	C14—C13—C18—C17	1.0 (4)
C7—C8—C9—N2	178.8 (3)	C7—C13—C18—C17	−179.8 (3)
C12—C8—C9—N1	−177.6 (2)	C16—C17—C18—C13	0.5 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N3^{i}	0.86	2.15	3.006 (4)	173

Symmetry codes: (i) −*x*+2, −*y*, −*z*.

Fig. 1

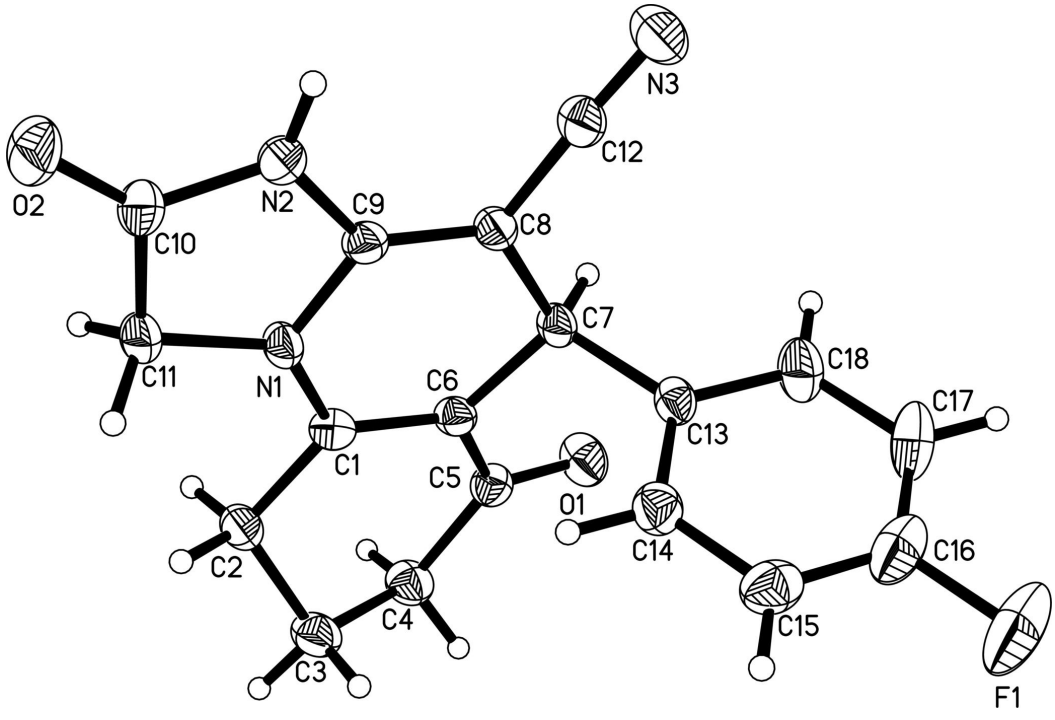
N3
C12
O2
N2
C9
C8
C10
C7
C18
C11
N1
C6
C17
C13
C1
C5
O1
C14
C16
C2
C4
C15
C3
F1

Fig. 2