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1-(4-{[8-(Trifluoromethyl)quinolin-4-yl]-amino}phenyl)ethanone

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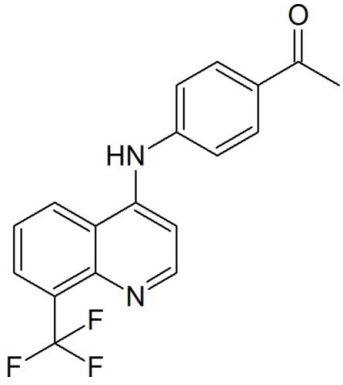
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.076; data-to-parameter ratio = 8.2.

In the title molecule, $C_{18}H_{13}F_3N_2O$, the mean planes of the quinolin-4-yl and phenylethanone groups are twisted, with a dihedral angle of 57.4 (1)°. In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules into zigzag chains running in the direction [011].

Related literature

For related structures, see: Lynch & McClenaghan (2001); Yathirajan *et al.* (2007). For related literature, see: Kucukguzel *et al.* (2000); Jung *et al.* (2002); Franck *et al.* (2004).



Experimental

Crystal data

$C_{18}H_{13}F_3N_2O$
M_r = 330.30
Orthorhombic, $Pna2_1$
a = 24.4690 (6) Å
b = 4.5342 (2) Å
c = 13.5408 (3) Å
V = 1502.32 (8) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 203 K
0.46 × 0.37 × 0.25 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.909, T_{max} = 1.000 (expected range = 0.707–0.778)
8038 measured reflections
1777 independent reflections
1657 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
S = 1.18
1777 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O1^{i}	0.87	2.08	2.901 (2)	158
C5—H5A···O1^{i}	0.94	2.54	3.436 (2)	159

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2279).

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supplementary materials

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1-(4-{[8-(Trifluoromethyl)quinolin-4-yl]amino}phenyl)ethanone

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Comment

In recent years fluorinated compounds find much importance in the pharmaceutical field. Fluorinated compounds in general, fluorinated heterocycles in particular, are those focused on much in modern-day medicinal chemistry. Incorporation of a fluorine atom instead of hydrogen one can alter the course of the reaction as well as its biological activities. Further introduction of a fluorine atom as the CF_3 group provides a more lipophilically and pharmacologically interesting compound compared to their non fluorinated analogues. The trifluoromethyl substituted compounds have been reported to possess biological activities as herbicides, fungicides and inhibitors for platelet aggregation. Quinolines are known to researchers for many years because a large number of natural products contain these heterocycles. They are found in numerous commericial products, including pharmaceuticals, fragrances and dyes. Quinoline alkaloids such as quinine, chloroquin, mefloquine and amodiaquine are used as efficient drugs for the treatment of malaria. Several quinoline derivatives have been evaluated *in vitro* against several parasites and HTLV-1 transformed cells. Prompted by the varied biological activities, the crystal structure of the title compound, $C_{18}H_{13}F_3N_2O$, (I), is here reported.

In (I) (Fig. 1), the mean planes of the quinolin-4-yl and phenyl-ethanone groups are twisted with a dihedral angle of 57.4 (1)°. In the crystal, intermolecular hydrogen bond interactions occur between N2–H2B and C5–H5A both to the same O1 (Table 1), which link the molecules into zigzag chains running in direction [011] (Fig. 2).

Experimental

A mixture of 4-chloro-8-(trifluoromethyl)quinoline (2.31 g, 0.01 mol), 1-(4-aminophenyl)ethanone, (1.35 g, 0.01 mol) and anhydrous potassium carbonate (2.76 g 0.02 mol) in 30 ml of dimethyl formamide (DMF) was heated over water bath for 6 h. The resulting mixture was filtered and the solution was concentrated on water bath to get the title compound. The crystals were obtained from acetone by slow evapoaration (*M*.p. 509 K). Elemental analysis found: C: 65.36; H: 3.94; N: 8.41%. $C_{18}H_{13}F_3N_2O$ requires C, 65.45, H, 3.97, N, 8.48%

Refinement

Atom H2B was located on a difference map, but placed in idealized position, N—H = 0.87 Å. C-bound H atoms were geometrically positioned, C—H = 0.94–0.97 Å. All H-atoms were refined as riding, with U_{iso}(H) = 1.2–1.5 U_{eq} of the parent atom. In the absence of any significant anomalous scatters in the molecule, 1777 Friedel pairs were merged before the final refinement.

Figures

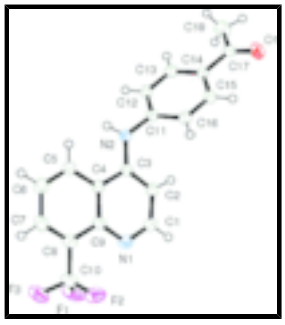

Fig. 1. Molecular structure of $C_{18}H_{13}F_3N_2O$, (I), showing atom labeling and 50% probability displacement ellipsoids.

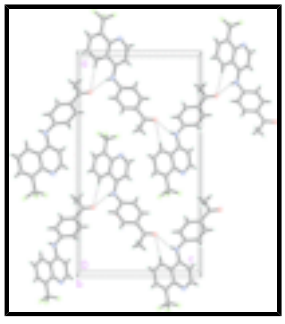

Fig. 2. Packing diagram of $C_{18}H_{13}F_3N_2O$ viewed down the *b* axis. Dashed lines indicate N–H···O and C–H···O hydrogen bonds.

1-(4-{[8-(Trifluoromethyl)quinolin-4-yl]amino}phenyl)ethanone

Crystal data

$C_{18}H_{13}F_3N_2O$	$D_x = 1.460$ Mg m^{-3}
$M_r = 330.30$	Cu *Kα* radiation λ = 1.54178 Å
Orthorhombic, *Pna*2$_1$	Cell parameters from 5931 reflections
a = 24.4690 (6) Å	θ = 4.7–32.5º
b = 4.5342 (2) Å	μ = 1.00 mm^{-1}
c = 13.5408 (3) Å	*T* = 203 K
V = 1502.32 (8) Å^3	Chunk, pale yellow
Z = 4	0.46 × 0.37 × 0.25 mm
$F_{000} = 680$	

Data collection

Oxford Diffraction Gemini R diffractometer	$R_{int} = 0.017$
Radiation source: fine-focus sealed tube	$\theta_{max} = 87.8$º
Monochromator: graphite	$\theta_{min} = 10.3$º
T = 203 K	*h* = −31→23
φ and ω scans	*k* = −5→5
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	*l* = −17→17
$T_{min} = 0.909$, $T_{max} = 1.000$	2 standard reflections

8038 measured reflections
1777 independent reflections
1657 reflections with $I > 2\sigma(I)$

every 50 reflections
intensity decay: none

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.076$

$S = 1.18$

1777 reflections

218 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.1154P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.010$

$\Delta\rho_{max} = 0.16$ e Å^{-3}

$\Delta\rho_{min} = -0.14$ e Å^{-3}

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.12637 (5)	0.0249 (3)	0.31930 (11)	0.0505 (3)
F2	0.13325 (5)	−0.3655 (3)	0.23050 (13)	0.0542 (4)
F3	0.14003 (5)	0.0597 (3)	0.16310 (11)	0.0522 (4)
O1	−0.30621 (6)	−0.7599 (4)	0.62756 (11)	0.0519 (4)
N1	0.03926 (6)	−0.4026 (4)	0.35402 (12)	0.0316 (3)
N2	−0.13031 (6)	−0.4360 (4)	0.29863 (11)	0.0368 (4)
H2B	−0.1408	−0.3692	0.2414	0.044*
C1	0.00518 (8)	−0.5549 (5)	0.40932 (15)	0.0331 (4)
H1A	0.0203	−0.6616	0.4622	0.040*
C2	−0.05134 (8)	−0.5721 (4)	0.39652 (14)	0.0321 (4)
H2A	−0.0727	−0.6860	0.4398	0.038*
C3	−0.07551 (7)	−0.4197 (4)	0.31947 (13)	0.0284 (4)
C4	−0.04056 (7)	−0.2480 (4)	0.25738 (12)	0.0259 (3)

C5	−0.06027 (8)	−0.0777 (4)	0.17722 (14)	0.0323 (4)
H5A	−0.0980	−0.0719	0.1643	0.039*
C6	−0.02561 (9)	0.0770 (5)	0.11878 (15)	0.0375 (5)
H6A	−0.0395	0.1882	0.0658	0.045*
C7	0.03120 (8)	0.0723 (5)	0.13691 (15)	0.0356 (4)
H7A	0.0549	0.1796	0.0958	0.043*
C8	0.05185 (8)	−0.0878 (4)	0.21401 (14)	0.0306 (4)
C9	0.01659 (7)	−0.2505 (4)	0.27749 (13)	0.0266 (3)
C10	0.11244 (8)	−0.0927 (4)	0.23199 (18)	0.0373 (4)
C11	−0.17126 (7)	−0.5504 (5)	0.36096 (13)	0.0316 (4)
C12	−0.21175 (7)	−0.7282 (5)	0.32065 (14)	0.0357 (4)
H12A	−0.2103	−0.7796	0.2535	0.043*
C13	−0.25430 (8)	−0.8302 (5)	0.37915 (14)	0.0348 (4)
H13A	−0.2815	−0.9505	0.3514	0.042*
C14	−0.25686 (7)	−0.7552 (5)	0.47883 (15)	0.0314 (4)
C15	−0.21584 (7)	−0.5776 (5)	0.51915 (13)	0.0363 (4)
H15A	−0.2171	−0.5275	0.5865	0.044*
C16	−0.17363 (8)	−0.4753 (5)	0.46115 (14)	0.0371 (5)
H16A	−0.1464	−0.3549	0.4889	0.045*
C17	−0.30242 (7)	−0.8529 (5)	0.54293 (15)	0.0367 (4)
C18	−0.34396 (9)	−1.0632 (6)	0.50333 (19)	0.0498 (6)
H18A	−0.3709	−1.1050	0.5540	0.075*
H18B	−0.3261	−1.2450	0.4838	0.075*
H18C	−0.3619	−0.9762	0.4465	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0364 (6)	0.0521 (8)	0.0630 (8)	−0.0090 (6)	−0.0096 (6)	−0.0003 (7)
F2	0.0363 (6)	0.0363 (6)	0.0902 (10)	0.0073 (5)	0.0131 (7)	0.0046 (8)
F3	0.0365 (6)	0.0493 (7)	0.0707 (9)	−0.0057 (6)	0.0151 (6)	0.0126 (7)
O1	0.0369 (7)	0.0842 (13)	0.0346 (7)	−0.0088 (8)	0.0094 (6)	0.0041 (8)
N1	0.0266 (7)	0.0337 (8)	0.0346 (8)	−0.0006 (7)	−0.0037 (6)	0.0004 (7)
N2	0.0250 (7)	0.0607 (12)	0.0246 (8)	−0.0036 (7)	−0.0007 (6)	0.0070 (8)
C1	0.0324 (8)	0.0370 (11)	0.0301 (8)	0.0016 (8)	−0.0053 (8)	0.0037 (8)
C2	0.0318 (8)	0.0368 (10)	0.0276 (8)	−0.0053 (8)	0.0001 (7)	0.0035 (8)
C3	0.0258 (8)	0.0363 (10)	0.0232 (7)	−0.0007 (7)	−0.0005 (7)	−0.0040 (8)
C4	0.0274 (7)	0.0279 (8)	0.0223 (7)	0.0012 (7)	0.0000 (6)	−0.0042 (7)
C5	0.0296 (8)	0.0367 (10)	0.0305 (9)	0.0037 (8)	−0.0017 (7)	0.0007 (8)
C6	0.0414 (10)	0.0376 (11)	0.0334 (9)	0.0051 (9)	0.0007 (8)	0.0077 (9)
C7	0.0377 (9)	0.0329 (10)	0.0363 (10)	−0.0010 (8)	0.0079 (8)	0.0048 (8)
C8	0.0302 (8)	0.0265 (9)	0.0353 (9)	−0.0006 (7)	0.0043 (7)	−0.0042 (8)
C9	0.0280 (7)	0.0249 (8)	0.0269 (8)	0.0007 (7)	0.0014 (7)	−0.0044 (7)
C10	0.0299 (9)	0.0296 (9)	0.0524 (12)	−0.0012 (8)	0.0052 (9)	0.0014 (10)
C11	0.0226 (8)	0.0461 (11)	0.0259 (8)	−0.0003 (8)	0.0007 (7)	0.0017 (8)
C12	0.0301 (8)	0.0528 (12)	0.0243 (8)	−0.0030 (9)	0.0002 (7)	−0.0027 (8)
C13	0.0286 (8)	0.0432 (11)	0.0326 (9)	−0.0044 (8)	−0.0027 (7)	−0.0018 (8)
C14	0.0235 (7)	0.0407 (10)	0.0299 (8)	0.0020 (8)	0.0010 (7)	0.0044 (8)

C15	0.0292 (9)	0.0555 (13)	0.0241 (8)	−0.0024 (9)	0.0008 (7)	−0.0027 (8)
C16	0.0284 (9)	0.0527 (13)	0.0303 (10)	−0.0077 (9)	−0.0006 (7)	−0.0050 (9)
C17	0.0272 (8)	0.0476 (11)	0.0352 (10)	0.0037 (8)	0.0010 (8)	0.0107 (9)
C18	0.0384 (10)	0.0592 (15)	0.0518 (13)	−0.0143 (11)	0.0038 (10)	0.0103 (11)

Geometric parameters (Å, °)

F1—C10	1.341 (3)	C7—C8	1.368 (3)
F2—C10	1.338 (2)	C7—H7A	0.9400
F3—C10	1.343 (2)	C8—C9	1.424 (3)
O1—C17	1.225 (3)	C8—C10	1.502 (3)
N1—C1	1.316 (3)	C11—C12	1.389 (3)
N1—C9	1.363 (2)	C11—C16	1.400 (3)
N2—C3	1.372 (2)	C12—C13	1.388 (3)
N2—C11	1.409 (2)	C12—H12A	0.9400
N2—H2B	0.8700	C13—C14	1.393 (3)
C1—C2	1.396 (3)	C13—H13A	0.9400
C1—H1A	0.9400	C14—C15	1.398 (3)
C2—C3	1.384 (3)	C14—C17	1.480 (3)
C2—H2A	0.9400	C15—C16	1.378 (3)
C3—C4	1.430 (2)	C15—H15A	0.9400
C4—C5	1.417 (3)	C16—H16A	0.9400
C4—C9	1.425 (2)	C17—C18	1.493 (3)
C5—C6	1.356 (3)	C18—H18A	0.9700
C5—H5A	0.9400	C18—H18B	0.9700
C6—C7	1.412 (3)	C18—H18C	0.9700
C6—H6A	0.9400		
C1—N1—C9	116.11 (15)	F2—C10—F3	105.89 (16)
C3—N2—C11	126.27 (15)	F1—C10—F3	106.28 (15)
C3—N2—H2B	116.9	F2—C10—C8	112.74 (16)
C11—N2—H2B	116.9	F1—C10—C8	112.83 (17)
N1—C1—C2	125.90 (18)	F3—C10—C8	112.08 (18)
N1—C1—H1A	117.0	C12—C11—C16	119.50 (18)
C2—C1—H1A	117.0	C12—C11—N2	119.05 (16)
C3—C2—C1	119.27 (17)	C16—C11—N2	121.36 (18)
C3—C2—H2A	120.4	C13—C12—C11	120.28 (17)
C1—C2—H2A	120.4	C13—C12—H12A	119.9
N2—C3—C2	123.06 (17)	C11—C12—H12A	119.9
N2—C3—C4	119.53 (16)	C12—C13—C14	120.37 (19)
C2—C3—C4	117.36 (16)	C12—C13—H13A	119.8
C5—C4—C9	119.01 (15)	C14—C13—H13A	119.8
C5—C4—C3	122.93 (15)	C13—C14—C15	119.11 (18)
C9—C4—C3	118.06 (15)	C13—C14—C17	121.93 (18)
C6—C5—C4	121.08 (17)	C15—C14—C17	118.95 (18)
C6—C5—H5A	119.5	C16—C15—C14	120.64 (17)
C4—C5—H5A	119.5	C16—C15—H15A	119.7
C5—C6—C7	120.45 (19)	C14—C15—H15A	119.7
C5—C6—H6A	119.8	C15—C16—C11	120.10 (18)
C7—C6—H6A	119.8	C15—C16—H16A	120.0

C8—C7—C6	120.29 (18)	C11—C16—H16A	120.0
C8—C7—H7A	119.9	O1—C17—C14	120.18 (19)
C6—C7—H7A	119.9	O1—C17—C18	120.28 (19)
C7—C8—C9	120.77 (17)	C14—C17—C18	119.54 (19)
C7—C8—C10	119.72 (17)	C17—C18—H18A	109.5
C9—C8—C10	119.51 (18)	C17—C18—H18B	109.5
N1—C9—C4	123.29 (16)	H18A—C18—H18B	109.5
N1—C9—C8	118.32 (16)	C17—C18—H18C	109.5
C4—C9—C8	118.38 (16)	H18A—C18—H18C	109.5
F2—C10—F1	106.50 (18)	H18B—C18—H18C	109.5
C9—N1—C1—C2	−0.3 (3)	C7—C8—C9—C4	1.5 (3)
N1—C1—C2—C3	0.2 (3)	C10—C8—C9—C4	−178.49 (16)
C11—N2—C3—C2	14.5 (3)	C7—C8—C10—F2	−122.3 (2)
C11—N2—C3—C4	−168.10 (19)	C9—C8—C10—F2	57.6 (3)
C1—C2—C3—N2	176.70 (19)	C7—C8—C10—F1	117.0 (2)
C1—C2—C3—C4	−0.8 (3)	C9—C8—C10—F1	−63.1 (2)
N2—C3—C4—C5	3.6 (3)	C7—C8—C10—F3	−2.9 (3)
C2—C3—C4—C5	−178.81 (18)	C9—C8—C10—F3	177.01 (16)
N2—C3—C4—C9	−176.21 (17)	C3—N2—C11—C12	−137.8 (2)
C2—C3—C4—C9	1.4 (2)	C3—N2—C11—C16	45.8 (3)
C9—C4—C5—C6	1.3 (3)	C16—C11—C12—C13	0.1 (3)
C3—C4—C5—C6	−178.56 (19)	N2—C11—C12—C13	−176.3 (2)
C4—C5—C6—C7	−0.2 (3)	C11—C12—C13—C14	0.0 (3)
C5—C6—C7—C8	−0.3 (3)	C12—C13—C14—C15	−0.4 (3)
C6—C7—C8—C9	−0.4 (3)	C12—C13—C14—C17	178.27 (19)
C6—C7—C8—C10	179.56 (19)	C13—C14—C15—C16	0.6 (3)
C1—N1—C9—C4	0.9 (3)	C17—C14—C15—C16	−178.1 (2)
C1—N1—C9—C8	−178.53 (18)	C14—C15—C16—C11	−0.4 (3)
C5—C4—C9—N1	178.66 (18)	C12—C11—C16—C15	0.1 (3)
C3—C4—C9—N1	−1.5 (2)	N2—C11—C16—C15	176.5 (2)
C5—C4—C9—C8	−1.9 (2)	C13—C14—C17—O1	−172.9 (2)
C3—C4—C9—C8	177.96 (17)	C15—C14—C17—O1	5.8 (3)
C7—C8—C9—N1	−179.05 (18)	C13—C14—C17—C18	6.5 (3)
C10—C8—C9—N1	1.0 (3)	C15—C14—C17—C18	−174.8 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···O1^{i}	0.87	2.08	2.901 (2)	158
C5—H5A···O1^{i}	0.94	2.54	3.436 (2)	159

Symmetry codes: (i) −*x*−1/2, *y*+1/2, *z*−1/2.

Fig. 1

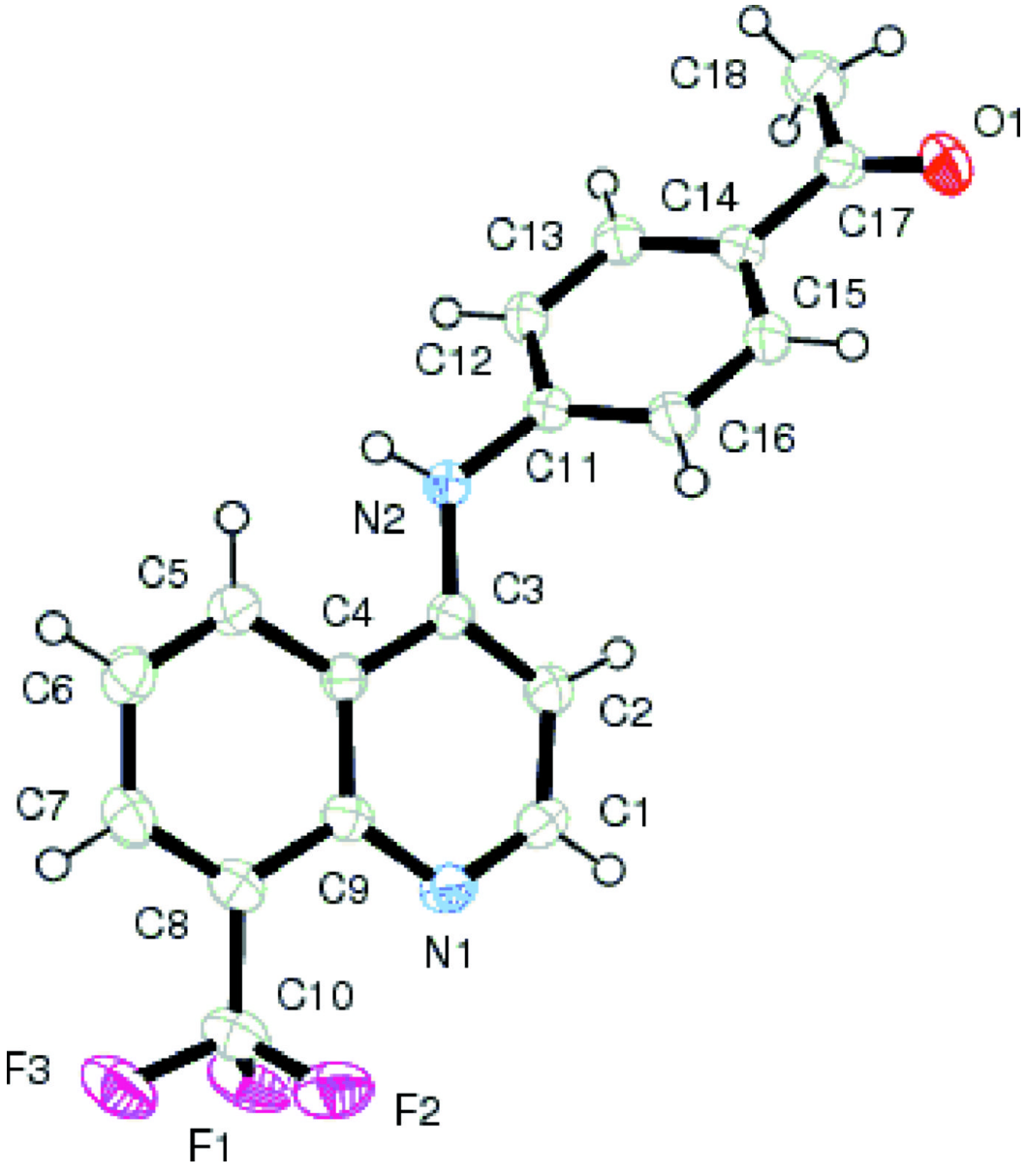
C18
O1
C14
C17
C13
C15
C12
C16
C11
N2
C5
C3
C4
C6
C2
C7
C1
C9
C8
N1
C10
F3
F2
F1

Fig. 2