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# (*R*)-1-{(2-Oxo-1,2-dihydroquinolin-6-yl)[3-(trifluoromethyl)phenyl]methyl}-1*H*-1,2,4-triazol-4-ium bromide

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**Key indicators**

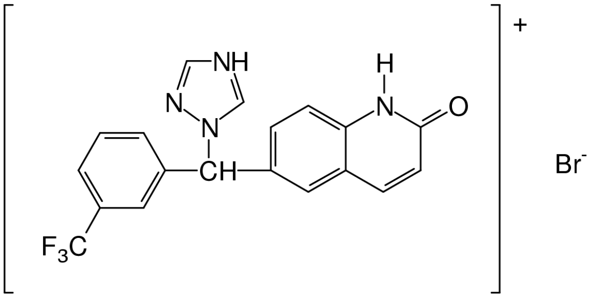
Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
*R* factor = 0.034
*wR* factor = 0.064
Data-to-parameter ratio = 12.0

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

The metabolism of all-*trans*-retinoic acid is mediated by a cytochrome dependent P-450 system. The title compound, $C_{19}H_{14}F_3N_4O^+\cdot Br^-$ (R111214), is an inhibitor of P-450. The three planar ring systems, *viz.* the triazolyl, phenyl and quinolinone groups, are arranged in a propeller-like fashion around the central CH group. The dihedral angles formed by the triazolyl/phenyl, triazolyl/quinolinone and phenyl/quinolinone planes are 55.8 (1), 79.85 (9) and 78.49 (9)°, respectively. The N—H···O hydrogen bonds, involving the triazolium N—H group and the quinolinone O atom, link the cations into infinite chains stretching along the *c* axis of the crystal.

## Comment

All-*trans*-retinoic acid (ATRA) is a metabolite of retinol (vitamin A) which is involved in growth and epithelial differentiation in mammals. However, the potency of ATRA is strongly attenuated by its rapid metabolism involving the stage of hydroxylation, mediated by a cytochrome dependent P-450 system (Leo *et al.*, 1989). The P-450 system is inhibited by the title compound, (I), which leads to increased plasma levels of ATRA.



(I)

The title compound has a propeller-like conformation (Fig. 1). The triazolyl and phenyl rings form an interplanar angle of 55.8 (1)° and the dihedral angles between these rings and the quinolinone moiety are 79.85 (9) and 78.49 (9)°, respectively. The small tilt between the planes of the six-membered rings in the quinolinone moiety is 1.67 (9)°. The bromide anion is hydrogen bonded to the quinolinone N atom. The N—H···O hydrogen bonds between the protonated nitrogen of the triazolyl ring and the quinolinone O atom link the cations into infinite chains stretching along the *c* axis of the crystal. Weaker C—H···Br and C—H···O hydrogen bonds also contribute to the stability of the crystalline product.

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Details of the hydrogen bonding geometry (D—H distances were not normalized) are given in Table 1.

## Experimental

The title compound was obtained from the Janssen Research Foundation, Beerse, Belgium. The synthesis has been described by Venet *et al.* (1996). Single crystals were grown by slow evaporation from a solution in ethanol.

### *Crystal data*

$C_{19}H_{14}F_3N_4O^+\cdot Br^-$
$M_r = 451.25$
Orthorhombic, $P2_12_12_1$
$a = 7.058$ (4) Å
$b = 16.212$ (8) Å
$c = 17.029$ (9) Å
$V = 1949$ (2) Å$^3$
$Z = 4$
$D_x = 1.538$ Mg m$^{-3}$
$D_m = 1.525$ Mg m$^{-3}$
$D_m$ measured by flotation in $CCl_4$/*n*-heptane
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
$\theta = 7.5$–$11.0°$
$\mu = 2.15$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.50 × 0.30 × 0.30 mm

### *Data collection*

Stoe Stadi-4 four-circle diffractometer
$\omega$ scans
Absorption correction: $\psi$ scan (*EMPIR*; Stoe & Cie, 1992)
$T_{min} = 0.427$, $T_{max} = 0.525$
5505 measured reflections
3463 independent reflections
2660 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.1°$
$h = -8 \rightarrow 8$
$k = -19 \rightarrow 19$
$l = -20 \rightarrow 20$
3 standard reflections
frequency: 60 min
intensity decay: 5.0%

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.064$
$S = 1.04$
3463 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.024P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ e Å$^{-3}$
Absolute structure: Flack (1983), 1457 Friedel pairs
Flack parameter = 0.000 (9)

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···Br | 0.86 | 2.46 | 3.293 (3) | 162 |
| N16—H16···O11$^{i}$ | 0.86 | 1.86 | 2.642 (4) | 150 |
| C17—H17···Br$^{ii}$ | 0.93 | 2.58 | 3.387 (4) | 145 |
| C15—H15···O11$^{iii}$ | 0.93 | 2.27 | 3.173 (5) | 163 |

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

After checking their presence in the difference map (which, in particular, unambiguously confirmed the protonation of the N1 and N16 atoms), H atoms were placed in geometrically calculated positions. All H atoms were allowed to ride on their parent atom. The isotropic displacement parameters were fixed at $1.2U_{eq}$ of their parent atoms. The $CF_3$ group shows a rotational disorder. It was modelled by two $CF_3$ groups with an occupation factor of 0.5 and refined using distance restraints.

Data collection: *DIF*4 (Stoe & Cie, 1992); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1992); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *PARST* (Nardelli, 1983).

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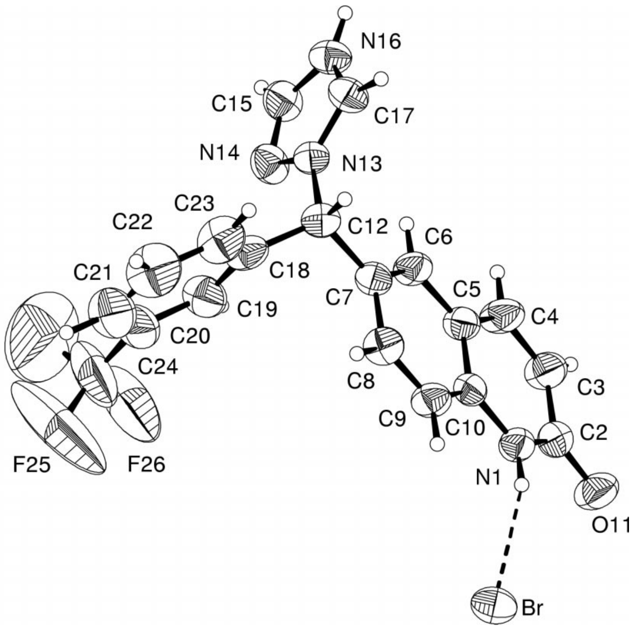

**Figure 1**
Perspective view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The alternative position of the disordered $CF_3$ group is not shown.