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# 1-(1-Ferrocenyl-1-methoxy-3-phenyl-2-propyl)-1*H*-1,2,4-triazole

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.007 Å
*R* factor = 0.042
*wR* factor = 0.108
Data-to-parameter ratio = 14.9

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



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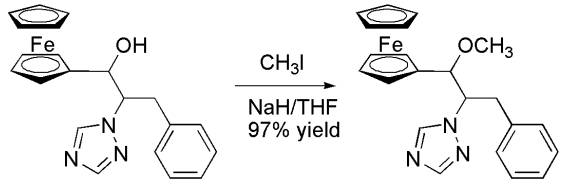
In a search for potent fungicidal agents, the title compound, $[Fe(C_5H_5)(C_{17}H_{18}N_3O)]$, has been synthesized and its single-crystal structure determined. It has proven that a bulky group, such as ferrocene, close to the triazole ring results in a decreased fungicidal activity.

## Comment

Due to its unique structure, different membrane-permeation properties and anomalous metabolism, ferrocene is often incorporated into organic compounds by chemists in order to obtain unexpected biological activity (Biot *et al.*, 2000; Sun *et al.*, 2002; Fang *et al.*, 2003*a*). A successful example is a ferrocene–chloroquine analogue, *viz.* ferrochloroquine {FQ: 7-chloro-4-[2-(*N*,*N*-dimethylaminomethyl)-*N*-ferrocenylmethylamino]quinoline}, in which one ferrocene unit is integrated into chloroquine (CQ) (Biot *et al.*, 1997). *In vitro*, FQ proved to be about 22 times more schizontocidal than CQ against chloroquine-resistant strains of *Plasmodium falciparum* and showed higher activity *in vivo* in mice infected with *P. Berghei* N and *P. yoelii* NS.




(I)

It is well known that compounds containing the 1*H*-1,2,4-triazole ring system are highly active as fungicides (Buchenauer, 1979), especially against the *Basidiomycete* and *Ascomycete* groups of fungi. Following our interest in a search for novel 1*H*-1,2,4-triazole compounds with potent fungicidal activities, we have sought to synthesize such 1*H*-1,2,4-triazole compounds incorporating ferrocenyl units.

Although these compounds are known to inhibit the biosynthesis of ergosterol in fungi, their structure–activity relationship (SAR) is not clear. From a study of the inhibition of ergosterol biosynthesis by 1-*tert*-butyl-2-(1,2,4-triazol-1-yl)-3-phenylpropan-1-ols, the structure of the cytochrome P-450–fungicide complex has been postulated and the fungicidal activity depends greatly on the stereochemistry of the non-N heterocyclic part of the molecule (Gadher *et al.*, 1983).

In order to determine the stereochemical features and structure–activity relationships of such triazole compounds, we investigated the crystal structure of a ferrocenyl-containing triazole compound, namely 1-(1-ferrocenyl-1-methoxy-3-

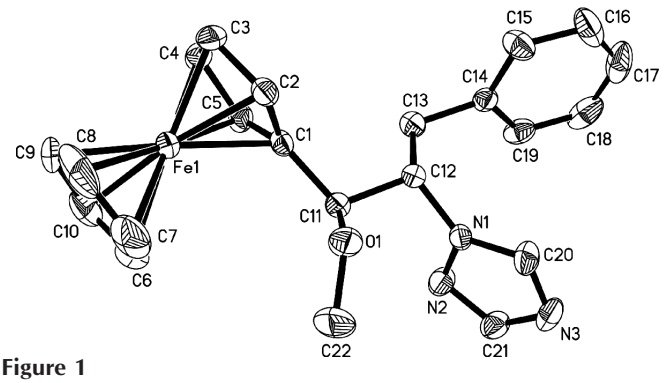



**Figure 1**
View of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

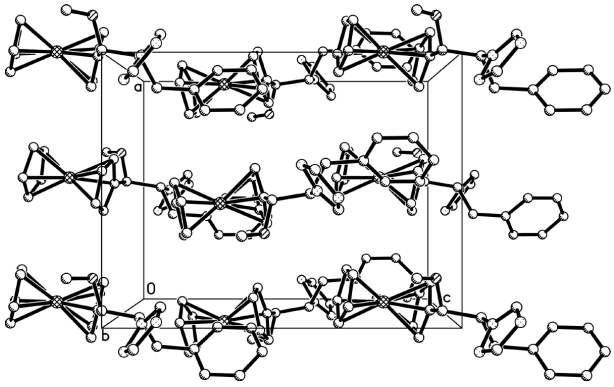



**Figure 2**
Packing diagram of the title compound. H atoms have been omitted for clarity.

phenylpropan-2-yl)-1*H*-1,2,4-triazole, (I), by single-crystal X-ray diffraction (Fig. 1).

To the best of our knowledge, a linkage between the triazole ring and the aryl group *via* a C—C single or double bond is essential for fungicidal activity. In addition, it has been proved that an extended carbon backbone linking the triazole ring and aryl group in an almost linear fashion possesses higher activity than a distorted backbone (Fang *et al.*, 2003*b*). The X-ray structure of (I) shows that, because of the bulkiness of ferrocene, the triazole ring and the aryl group are not connected in such a way, but *via* a bent linkage (Fig. 1), and the compound does not display fungicidal activity. This may imply that a bulky group close to the triazole ring is not a wise choice for the generation of compounds with fungicidal activity.

The title compound contains four planar groups: (i) the substituted cyclopentadienyl ring composed of atoms C1–C5, (ii) the cyclopentadienyl ring composed of atoms C6–C10, (iii) the C14–C19 benzene ring and (iv) the triazole ring composed of atoms N1/N2/C21/N3/C20. The dihedral angles between planes i and iv and between planes iii and iv are 25.4 (2) and 47.7 (2)°, respectively.

## Experimental

The title compound was prepared by the reaction of 1-(1-ferrocenyl-1-hydroxy-3-phenylpropan-2-yl)-1*H*-1,2,4-triazole with methyl iodide in the presence of sodium hydride (Jin *et al.*, 2004). It was recrystallized from diethyl ether and petroleum ether (1/1 *v*/*v*) to give yellow crystals.

*Crystal data*

$[Fe(C_5H_5)(C_{17}H_{18}N_3O)]$
$M_r$ = 401.28
Orthorhombic, $Pca2_1$
$a$ = 10.165 (5) Å
$b$ = 14.205 (7) Å
$c$ = 13.262 (6) Å
$V$ = 1915.0 (16) Å$^3$
$Z$ = 4
$D_x$ = 1.392 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 840 reflections
$\theta$ = 2.5–22.4°
$\mu$ = 0.80 mm$^{-1}$
$T$ = 293 (2) K
Prism, yellow
0.32 × 0.25 × 0.20 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.715, $T_{max}$ = 0.851
10 319 measured reflections
3690 independent reflections
2665 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049
$\theta_{max}$ = 26.5°
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 17$
$l = -16 \rightarrow 13$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
$S$ = 1.06
3690 reflections
247 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0036 (6)
Absolute structure: Flack (1983), 1619 Friedel pairs
Flack parameter = 0.02 (3)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Fe1—C9 | 2.014 (5) | C2—C3 | 1.410 (7) |
| Fe1—C1 | 2.043 (4) | C2—H2 | 0.9300 |
| N1—C20 | 1.324 (5) | C6—C7 | 1.399 (4) |
| N1—N2 | 1.351 (5) | C11—C12 | 1.531 (5) |
| N1—C12 | 1.453 (5) | C12—C13 | 1.526 (6) |
| N2—C21 | 1.306 (6) | C13—C14 | 1.505 (6) |
| N3—C20 | 1.295 (6) | C14—C15 | 1.371 (6) |
| N3—C21 | 1.332 (6) | C14—C19 | 1.371 (6) |
| O1—C11 | 1.410 (5) | C15—C16 | 1.385 (8) |
| C1—C11 | 1.501 (6) | | |
| C1—Fe1—C2 | 40.61 (17) | N1—C12—C11 | 109.0 (3) |
| C2—C1—C11 | 126.3 (4) | C14—C13—C12 | 110.7 (4) |
| C1—C2—Fe1 | 69.4 (3) | C15—C14—C13 | 120.9 (4) |
| O1—C11—C1 | 110.1 (3) | N3—C20—N1 | 112.2 (4) |
| O1—C11—C12 | 107.0 (3) | | |
| C20—N1—N2—C21 | 0.5 (5) | C20—N1—C12—C11 | −121.5 (5) |
| C12—N1—N2—C21 | 178.2 (4) | N2—N1—C12—C11 | 61.3 (5) |
| C8—Fe1—C1—C5 | 177.3 (4) | O1—C11—C12—N1 | 68.6 (4) |
| C7—Fe1—C1—C5 | 143.4 (5) | C1—C11—C12—N1 | −171.0 (3) |
| C5—C1—C2—C3 | 0.7 (5) | O1—C11—C12—C13 | −166.2 (3) |
| C11—C1—C5—C4 | −175.6 (4) | N1—C12—C13—C14 | −57.9 (5) |
| C2—C1—C11—C12 | −85.3 (5) | C11—C12—C13—C14 | 177.6 (4) |
| C5—C1—C11—C12 | 88.8 (5) | C21—N3—C20—N1 | 0.2 (6) |
| Fe1—C1—C11—C12 | −178.9 (3) | N2—N1—C20—N3 | −0.4 (6) |
| C20—N1—C12—C13 | 109.9 (5) | C12—N1—C20—N3 | −177.9 (4) |
| N2—N1—C12—C13 | −67.3 (5) | N1—N2—C21—N3 | −0.4 (6) |

All H atoms were placed in calculated positions, with C—H = 0.93–0.98 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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