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# 5-(2-Hydroxyphenyl)-4-(4-methoxyphenyl)-3-(4-methylphenyl)-4*H*-1,2,4-triazole

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**Key indicators**

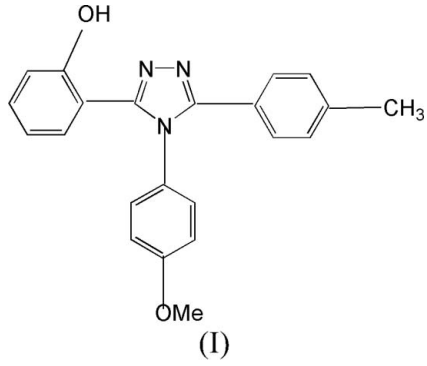
Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.041
*wR* factor = 0.129
Data-to-parameter ratio = 17.9

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

In the title compound, $C_{22}H_{19}N_3O_2$, there are two independent molecules in the asymmetric unit. Intramolecular O—H···N hydrogen bonds are observed in the crystal structure.

## Comment

Recently, we reported the syntheses and structures of some 1,2,4-triazole ligands and their metal complexes (Zhang *et al.*, 2004; Zhang, Liu, Ma *et al.*, 2005; Zhang, Liu, Yang *et al.*, 2005; Zhang, Liu & Shao, 2006; Zhang, Liu, Chen *et al.*, 2006). As an extension of our work on the structural characterization of triazole derivatives, we report here the crystal structure of the title compound, (I).




(I)

The asymmetric unit of (I) consists of two independent molecules of 4-(4-methoxyphenyl)-3-(4-methylphenyl)-5-(2-hydroxyphenyl)-4*H*-1,2,4-triazole (Fig. 1). In both molecules, the bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The dihedral angles formed by the triazole ring with the aromatic ring of the hydroxyphenyl, methylphenyl and methoxyphenyl groups are 15.13 (5), 31.00 (5) and 77.54 (4)°, respectively, in one molecule, and 5.25 (7), 58.71 (7) and 83.09 (6)°, respectively, in the other molecule.

The crystal structure is stabilized by intramolecular O—H···N hydrogen bonds (Table 1).

## Experimental

The title compound was synthesized according to the literature method of Zhu *et al.* (2000). Equivalent amounts of *p*-methoxyphosphazoanilide (0.2743 g) and *N*-2-hydroxyphenyl-*N*′-4-methylphenylhydrazine (0.2703 g) were reacted in ethanol (10 ml) for 1 h. After allowing the resulting solution to stand in air for 15 d, colourless block-shaped crystals were formed on slow evaporation of the solvent.

*Crystal data*

$C_{22}H_{19}N_3O_2$
$M_r$ = 357.40
Triclinic, $P\overline{1}$
$a$ = 9.5954 (4) Å
$b$ = 12.4637 (5) Å
$c$ = 15.8750 (6) Å
$\alpha$ = 90.9566 (6)°
$\beta$ = 103.2093 (6)°
$\gamma$ = 90.4278 (6)°
$V$ = 1847.95 (13) Å$^3$
$Z$ = 4
$D_x$ = 1.285 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 298 (2) K
Block, colourless
0.18 × 0.16 × 0.11 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.985, $T_{max}$ = 0.991
22546 measured reflections
8963 independent reflections
4446 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023
$\theta_{max}$ = 28.3°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.129
$S$ = 0.95
8963 reflections
500 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.019
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.12 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 1997*a*)
Extinction coefficient: 0.0081 (12)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N2 | 0.946 (15) | 1.716 (17) | 2.5932 (18) | 153 (2) |
| O3—H2···N5 | 0.902 (16) | 1.745 (19) | 2.547 (3) | 147 (2) |

The hydroxy H atoms were located in a difference map and refined freely. The remaining H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C), or 1.5$U_{eq}$(C) for methyl H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

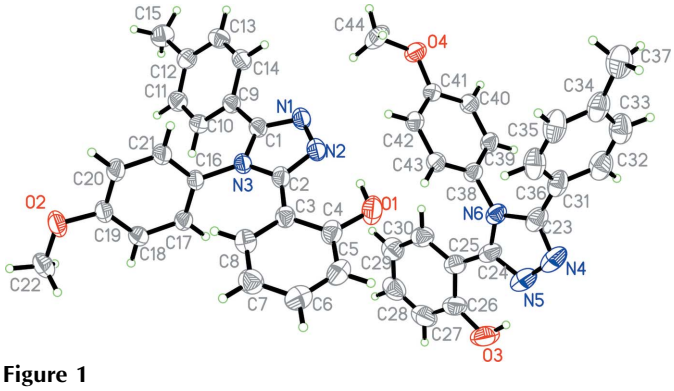



**Figure 1**
The asymmmetric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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