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[3-(2-Hydroxyphenyl)-5-phenyl-4,5-dihydropyrazol-1-yl](pyridin-3-yl)methanone

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Key indicators

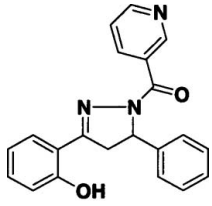
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.107
Data-to-parameter ratio = 15.9

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

In the title compound, $C_{21}H_{17}N_3O_2$, the dihedral angles between the central pyrazole and the substituent pyridine, hydroxyphenyl and benzene rings are 48.58 (1), 5.2 (1) and 84.73 (1)°, respectively.

Comment

Pyrazole derivatives have been identified as inhibitors of monoamine oxidase (MAO; Chimenti *et al.*, 2004, 2005). MAO inhibitors are important for the treatment of several psychiatric and neurological diseases. MAO-B inhibitors are coadjuvant in the treatment of Parkinson's disease (Cesura & Pletscher, 1992) and also Alzheimer's disease (Saura *et al.*, 1994). MAO-A inhibitors are used as antidepressant and anti-anxiety drugs (Amrein *et al.*, 1999). In order to seek out selective inhibitors of monoamine oxidase, we have started to construct a library of pyrazole derivatives. The title compound, (I), was thus synthesized and its crystal structure is presented here.



(I)

All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The dihedral angles between the central pyrazole and the substituent pyridine, hydroxyphenyl and benzene rings are 48.58 (1), 5.2 (1) and 84.73 (1)°, respectively. An intramolecular O1—H1···N1 hydrogen bond [H1···N1 = 1.90 Å, O1···N1 = 2.636 (2) Å and O1—H1···N1 = 145°] between the OH group of the hydroxyphenyl ring and atom N1 of the pyrazole ring locks the two rings into an essentially coplanar conformation. The crystal packing shows no unusually close intermolecular contacts.

Experimental

1-(2-Hydroxyphenyl)-3-phenylprop-2-en-1-one (112.0 mg, 0.5 mmol) and nicotinic acid hydrazide (69.0 mg, 0.5 mmol) were dissolved in propan-2-ol (2 ml). This solution was heated for 2 h at 473 K through the use of microwave irradiation. After cooling to room temperature, the precipitate was collected by filtration and dried, to give the title compound as a colorless solid (70.0 mg, 42.9%). The resultant solid was crystallized from ethanol to afford crystals of (I) suitable for X-ray analysis.

Crystal data

$C_{21}H_{17}N_3O_2$
M_r = 343.38
Monoclinic, $P2_1/c$
a = 5.9050 (10) Å
b = 19.840 (3) Å
c = 14.283 (2) Å
β = 97.516 (3)°
V = 1659.0 (4) Å^3
Z = 4
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
Cube, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.982
13968 measured reflections
3742 independent reflections
2687 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
S = 1.02
3742 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.1984P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.95–1.00 Å, O—H = 0.84 Å and U_{iso}(H) = 1.2U_{eq}(C,O).

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-32* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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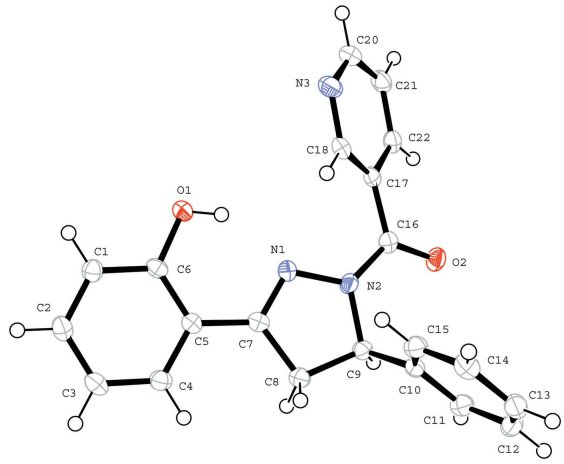

Figure 1
The molecular structure of the title compound, (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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