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2-(4-Hydroxy-3-methoxyphenyl)-1-phenethyl-1,2-dihydroquinazolin-4(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.193
Data-to-parameter ratio = 17.0

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

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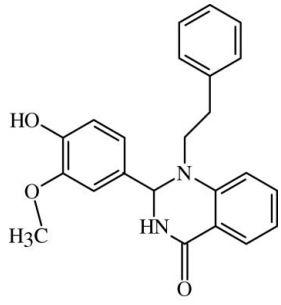
In the crystal structure of the title compound, $C_{23}H_{22}N_2O_3$, the dihydropyrimidine (DHPM) ring adopts a sofa conformation. The methoxy-substituted benzene ring is oriented equatorially and the phenylethyl group has a fully extended conformation with respect to the DHPM ring. Four adjacent molecules are linked *via* N—H···O and O—H···O hydrogen-bonding interactions, generating a tetrameric unit. The crystal structure is further stabilized by C—H···π(arene) interactions.

Comment

Quinazolin-4(1*H*)-ones, commonly known as benzopyrimidones, represent an important class of heterocyclic compounds. Furthermore, 2,3-dihydro-1*H*-quinazolin-4-one derivatives are of biological and pharmaceutical importance (Bonola *et al.*, 1968, Levin *et al.*, 1994, Okumura *et al.*, 1968). Structural analysis of these compounds provides an opportunity to study the biological activity and its implication for the structural requirement needed for binding to the receptors. It has been observed and reported by us (Swamy & Ravikumar, 2005) that substitution at the C-2 position in the DHPM ring plays a crucial role in the ring conformation. In other words, the bulkiness of the substituent appears to be a necessary condition for the dihydropyrimidine (DHPM) ring to adopt a sofa conformation. In a continuation of our studies on the influence of substituents on the ring (DHPM) conformation, we have undertaken this study and report here the structural details of the title compound, (I).



(I)

The geometric parameters within the DHPM ring of (I) are affected by conjugation. The formal single bonds N1—C5 and N2—C3 have partial double-bond character (Table 1) (Burke-Laing & Laing, 1976). Furthermore, the sum of the angles around atoms N1 and N2 are 360.0 and 351.2°, respectively, indicating sp^2 hybridization. The lengthening of the C5—O2 bond [1.237 (3) Å] from the normal C=O distance (1.20 Å) could be attributed to some conjugation involving atom O2 (Tiekink, 1989). The DHPM ring is puckered in such a manner

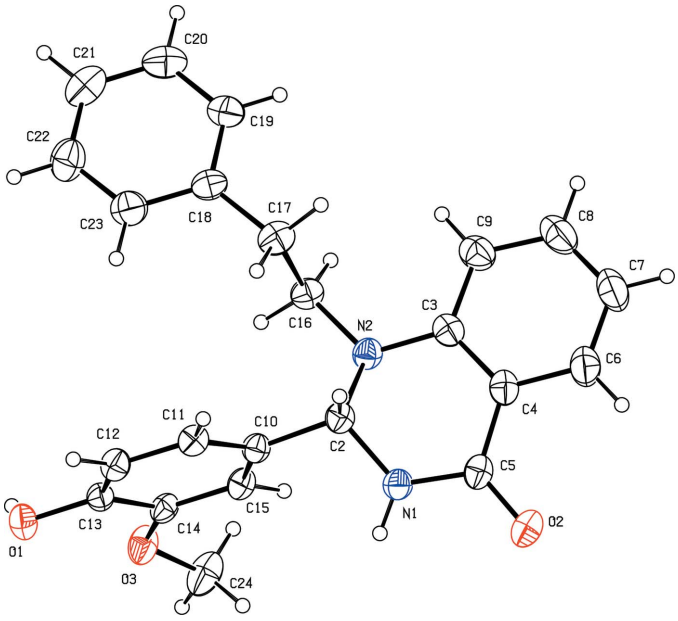


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

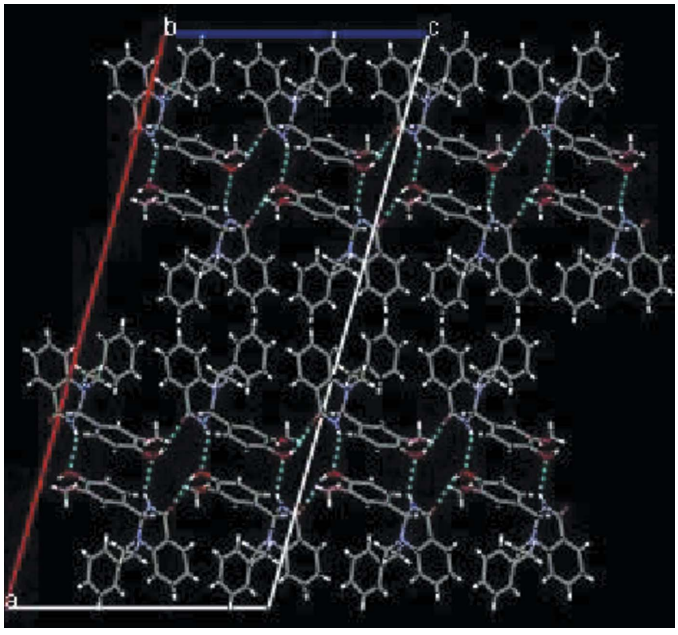


Figure 2
Crystal structure of (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

that atoms N1, C3, C4, C5 and N2 are coplanar (maximum deviation of 0.045 Å from the mean plane), with the sixth atom, C2, displaced 0.595 (2) Å above the least-squares plane. Analysis of the torsion angles (Table 1) indicates that the DHPM ring in (I) is in a distorted sofa conformation [ΔC_s(C2)=17.7°]. A literature survey (Chandra Mohan *et al.*, 2003) reveals that there is an apparent correlation between the pharmacological activity of such compounds and the planarity of the DHPM ring. Precisely, the activity of such compounds increases with increasing planarity of the hetero ring. In the present case, Θ_{av} (the average of C2—N2—C3—C4 and C2—N1—C5—C4) is 21.8 (3)°.

The methoxy group is not in the plane of the benzene ring to which it is attached (Table 1); the torsion angle N2—C16—C17—C18 is 174.5 (2)°. Benzene ring C18–C23 is nearly coplanar with the DHPM ring, whereas benzene ring C10–C15 is nearly perpendicular to the DHPM ring [dihedral angle = 87.1 (1)°].

In the crystal structure, molecules are connected *via* N—H···O and O—H···O hydrogen bonds (Table 2) into $R_2^2(12)$-type rings (Bernstein *et al.*, 1995), which are further connected into chains by hydrogen bonds. In addition, the structure is further stabilized by C—H···O and C—H···π(arene) interactions.

Experimental

The title compound, (I), was prepared according to a literature procedure (Sadanandam *et al.*, 1992) and was recrystallized from methanol.

Crystal data

$C_{23}H_{22}N_2O_3$
M_r = 374.43
Monoclinic, $C2/c$
a = 36.113 (5) Å
b = 6.8124 (9) Å
c = 15.931 (2) Å
β = 105.504 (2)°
V = 3776.7 (9) Å^3
Z = 8
D_x = 1.321 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1838 reflections
θ = 2.3–22.7°
μ = 0.09 mm^{-1}
T = 273 (2) K
Block, colourless
0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
11047 measured reflections
4349 independent reflections
2519 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 28.0°
$h = -39 \rightarrow 45$
$k = -8 \rightarrow 8$
$l = -20 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.193
S = 1.00
4349 reflections
256 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1049P)^2 + 0.0523P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C3—N2	1.395 (3)	C5—N1	1.342 (3)
N2—C3—C4—C6	179.2 (2)	C4—C3—N2—C2	29.1 (3)
C3—C4—C5—N1	−12.7 (3)	N1—C2—N2—C3	−51.4 (2)
C4—C5—N1—C2	−14.4 (3)	C15—C14—O3—C24	12.2 (4)
N2—C2—N1—C5	45.5 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1′···O1^{i}	0.86	2.24	2.952 (3)	140
O1—H1···O2^{ii}	0.82	1.97	2.734 (2)	154
C11—H11···O2^{iii}	0.93	2.65	3.564 (3)	167
C7—H7···*Cg*1^{iv}	0.93	3.01	3.78	141
C12—H12···*Cg*2^{v}	0.93	2.85	3.62	142

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+1, z+\frac{1}{2}$; (iii) $x, y+1, z$; (iv) $-x+\frac{1}{2}, y+\frac{3}{2}, -z-\frac{1}{2}$; (v) $x, -y, z-\frac{1}{2}$. Note: *Cg*1 is the centroid of the C10–C15 ring and *Cg*2 is the centroid of the C18–C23 ring.

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, N—H = 0.86 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.5U_{eq}(C,O) for methyl, imino (–NH–) and hydroxy H atoms, and 1.2U_{eq}(C) for other H atoms. The OH group was allowed to rotate but not to tip relative to the C—O bond.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bonola, G., Da Re, P., Magistretti, M. J., Massarani, E. & Setnikar, I. (1968). *J. Med. Chem.* **11**, 1136–1139.
Burke-Laing, M. & Laing, M. (1976). *Acta Cryst.* B**32**, 3216–3224.
Bruker (2001). *SAINT* (Version 6.28a) and *SMART* (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
Chandra Mohan, K., Ravikumar, K., Shetty, M. M. & Velmurugan, D. (2003). *Z. Kristallogr.* **218**, 46–55.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Levin, J. I., Chan, P. S., Bailey, T., Katocs, A. S. Jr & Venkatesan, A. M. (1994). *Bioorg. Med. Chem. Lett.* **4**, 1141–1146.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Okumura, K., Oine, T., Yamada, Y., Hayashi, G. & Nakama, M. (1968). *J. Med. Chem.* **11**, 348–352.
Sadanandam, Y. S., Shetty, M. M. & Diwan, P. V. (1992). *Eur. J. Med. Chem.* **27**, 87–92.
Sheldrick, G. M. (1997). *SHELXS97* AND *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Swamy, G. Y. S. K. & Ravikumar, K. (2005). *J. Chem. Crystallogr.* **3**, 183–189.
Tiekink, E. R. T. (1989). *Z. Kristallogr.* **187**, 79–84.