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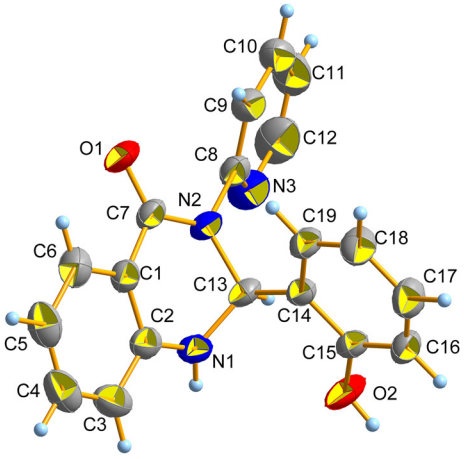
The crystal structure of 2-(2-hydroxyphenyl)-3-(pyridin-2-yl)-2,3- dihydroquinazolin-4(1*H*)-one, $C_{19}H_{15}N_3O_2$



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Abstract

$C_{19}H_{15}N_3O_2$, orthorhombic, $P2_12_12_1$ (no. 19), a = 8.8676(14) Å, b = 10.8842(17) Å, c = 16.167(3) Å, V = 1560.3(4) Å^3, Z = 4, $R_{gt}(F)$ = 0.0305, $wR_{ref}(F^2)$ = 0.0828, T = 296(2) K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.46 × 0.41 × 0.35 mm
Wavelength:	Mo$K\alpha$ radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker Apex-II, φ and ω-scans
θ_{max}, completeness:	25°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14903, 2753, 0.016
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs}°>°2σ(I_{obs}), 2,662
$N(param)_{refined}$:	219
Programs:	Bruker programs,[1] Shelx,[2,3] Olex2[4]

1 Source of material

Salicylaldehyde (0.244 g, 2 mmol) and 2-amino-*N*-(pyridin-2-yl) benzamide (0.426 g, 2 mmol) were dissolved in ethanol (20 mL) and the mixture was refluxed for 6 h. The reaction mixture was concentrated in vacuum, and the title compound was isolated through a silica gel column chromatography (PE:EtOAc = 4:1) as a white solid (0.349 g, 55 % yield). The single crystal of the product was obtained by recrystallization from ethanol through slow evaporation within one week.

2 Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The U_{iso} values of the phenolic hydroxyl were set to 1.5 U_{eq} (C), and the U_{iso} values of all other hydrogen atoms were set to 1.2 U_{eq} (C).

3 Discussion

2,3-Dihydroquinazolin-4(1*H*)-ones have attracted the attention of pharmaceutical chemists due to their diverse biological activities.[5,6] Because their structures contain chiral carbon atoms, their structures are also the focus of research.[7–9]

Herein, a new 2,3-dihydroquinazolin-4(1*H*)-one compound was synthesized and characterized by single-crystal X-ray diffraction.[1–4] The crystal structure reveals that C(13) atom is sp^3 hybridized and chiral carbon. Plane I (C1–C6) forms a dihedral angle of 31.813(1)° with plane II (C8–N3), and 89.133(2)° with plane III (C14–C19). The dihedral angle

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between plane II and plane III is 79.387(2)°. The bond lengths of O(1)–C(7), C(1)–C(7) and C(15)–O(2) are 1.233(2) Å, 1.481(3) Å and 1.361(3) Å. The C(13)–N(1), C(13)–N(2) and C(8)–N(2) bond lengths are 1.446(3) Å, 1.473(2) Å and 1.435(3) Å, which are longer than (C2)–N(1), C(7)–N(2), C(8)–N(3), C(12)–N(3) bond lengths of 1.380(3) Å, 1.359(3) Å, 1.322(3) Å, 1.346(4) Å, respectively.

All geometric parameters are in the xpected ranges.[8–10]

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References

1. Bruker. Apex3, Saint-Plus, Xprep; Bruker AXS Inc.: Madison, Wisconsin, USA, 2016.
2. Sheldrick, G. M. Shelxt – Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallogr.* **2015**, *A71*, 3–8.
3. Sheldrick, G. M. Crystal Structure Refinement with Shelxl. *Acta Crystallogr.* **2015**, *C71*, 3–8.
4. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A.; Puschmann, H. Olex2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.
5. Shi, D.; Li, Z.; Shi, C.; Zhuang, Q.; Zhang, Y. 3-(4-Bromo-phenyl)-2,2-dimethyl-2,3-Dhydro-quinazolin-4(1*H*)-one. *Acta Cryst.* **2004**, *E60*, o1992–o1994.
6. Patel, N. B.; Patel, J. C. Synthesis and Antimicrobial Activities of 2-Azetidinyl-4-Quinazolinone Derivatives of Diclofenac Analogue. *Med. Chem. Res.* **2001**, *20*, 511–521.
7. Amnerkar, N. D.; Bhusari, K. P. Synthesis, Anticonvulsant Activity and 3D-QSAR Study of Some Prop-2-Eneamido and 1-Acetyl-pyrazolin Derivatives of Aminobenzothiazole. *Eur. J. Med. Chem.* **2010**, *45*, 149–159.
8. Liu, S.-J.; Zhang, Y.; Yuan, L.; Chen, X.-M. The Crystal Structure of 2,3-Di(pyridin-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one, $C_{18}H_{14}N_4O$. *Z. Kristallogr. NCS* **2024**, *239*, 1001–1002.
9. Butcher, R. J.; Jasinski, J. P.; Narayana, B.; Sunil, K.; Yathirajan, H. S. 2-(4-Chlorophenyl)-3-{[(1*E*)-(4-chlorophenyl) methylene]amino}-2,3-dihydroquinazolin-4(1*H*)-one. *Acta Cryst.* **2007**, *E63*, o4025–o4026.
10. Memarian, H. R.; Ebrahimi, S.; Rudbari, H. A.; Sabzyan, H.; Nardo, V. M. Inter- and Intramolecular Interactions in 2,3-Dihydroquinazolin-4(1*H*)-Ones: Molecular Structure and Conformational Analysis. *J. Iran. Chem. Soc.* **2016**, *13*, 1395–1404.