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Supporting Information

Functionalization of gold nanoparticles with two aminoalcohol-based quinoxaline derivatives for targeting phosphoinositide 3-kinases (PI3Kα).

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X-Ray crystallography

A prismatic colorless crystal with dimensions of 0.32 x 0.24 x 0.18 mm^3 was selected from a crystalline sample of the compound OAQX for crystallographic analysis. X-ray diffraction data were measured on a Kappa APEXII Duo diffractometer. The frames were recorded with ω and ϕ scans. Collected intensities were corrected for Lorentz and polarization effects. No absorption correction was applied to measured data. The structure was solved by direct methods and refined by full-matrix least-squares methods using SIR97[1] and SHELXL97[2] programs, respectively. All non-hydrogen atoms were refined anisotropically. H atoms attached to C atoms were placed at their idealized positions, with C-H distances and U_{eq} values taken from the default settings of the refinement program. H atom of the alcohol group was found from Fourier difference map and refined isotropically as free atom. Ortep plot was drawn using PLATON[3] software. Selected crystallographic data are shown in Table 1 and full crystallographic tables for compound OAQX have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 1038640. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

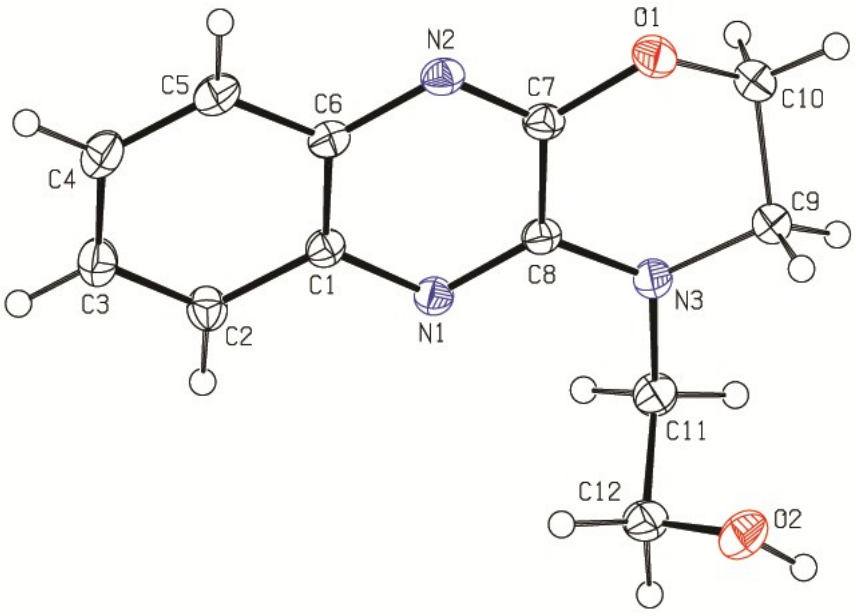

Table 1. Crystal data and structure refinement for compound OAQX.

Empirical formula	$C_{12}H_{13}N_3O_2$
Formula weight	231.25
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2_1/n
Unit cell dimensions	a = 10.1217(2) Å
	b = 9.5662(2) Å
	c = 11.2210(3) Å
	β = 98.633(2)°
Volume	1074.18(4) $Å^3$
Z	4
Density (calculated)	1.430 Mg/m^3
Absorption coefficient	0.101 mm^{-1}
F(000)	488
Crystal size	0.32 x 0.24 x 0.18 mm^3
Theta range for data collection	2.53 to 33.21°
Index ranges	-15 ≤ h ≤ 15, -13 ≤ k ≤ 14, -17 ≤ l ≤ 10
Reflections collected	9418
Independent reflections	4090 (R_{int} = 0.0175)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4090 / 0 / 173
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0430, wR2 = 0.1264
R indices (all data)	R1 = 0.0530, wR2 = 0.1357
Largest diff. peak and hole	0.458 and -0.199 e.$Å^{-3}$

References

1. Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G. L.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *J. Appl. Crystallogr*. **1999**, *32*, 115.

2. Herbst-Irmer, R.; Sheldrick, G. M.; *Acta Crystallogr., Sect. B: Struct. Sci.* **1998**, *54*, 443.

3. Spek, A. L.; *J. Appl. Crystallogr*. **2003**, *36*, 7.