Synthesis of Piperazine Tethered 4-Aminoquinoline-Pyrimidine Hybrids as Potent Antimalarial Agents

Supporting Information

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Crystallographic Data

The crystallization was achieved by the slow evaporation of solution of crude compound in $CHCl_3$ which afforded highly crystalline compound (**4a**). Diffraction data of compound **4a** were collected on an Oxford CCD diffractometer having Xcalibur, sapphire diffraction measurement device at 293 K, using graphite-monochromated Mo-Ka radiation ($\lambda = 0.71073$ Å) (1). The multi-scan absorption correction was applied using CrysalisPRO. The crystal structures were solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on F^2 using SHELXL97. Hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using WinGX software (2). CCDC 984609 contains the supplementary crystallographic data for compound **4a**. The crystallographic data collection and structure refinement parameters forall complexes are summarized in table 1. 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: X-ray crystallographic data collection and structure refinement parameters for compound **4a**

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	Compound **4a**
Molecular formula	$C_{17}H_{15}Cl_2N_5$
FW	360.24
T(K)	298(2)
Crystal system	Monoclinic
Space group	*P 21/c*
A	7.8252(6)
B	11.7133(7)

C	18.1164(13)
α	90
β	100.744(7)
γ	90
V (Å3)	1631.4(2)
Z	4
d (g cm-3)	1.467
F (000)	744
Goodness of fit (F2)	1.087
R1, wR$_2$ [I >2 (I)]	0.0398, 0.0953
R1, wR$_2$ [all data][a]	0.0484, 0.0997

[a] $R_1 = \Sigma ||Fo| - |Fc||/\Sigma|Fo|$; $wR_2 = \{\Sigma[w(/Fo/^2 - /Fc/^2)^2]/\Sigma[wFo^4]\}^{1/2}$

Table 2: Selected bond lengths [Å] for compound **4a.**

Bond lengths	
Cl(1)-C(1)	1.739(2)
Cl(2)-C(17)	1.750(2)
N(1)-C(3)	1.367(3)
N(1)-C(7)	1.310(3)
N(2)-C(9)	1.410(2)
N(2)-C(10)	1.455(2)
N(2)-C(13)	1.474(2)
N(3)-C(11)	1.458(3)
N(3)-C(12)	1.455(2)
N(3)-C(14)	1.351(2)
N(4)-C(14)	1.352(3)
N(4)-C(17)	1.314(2)
N(5)-C(16)	1.352(3)
N(5)-C(17)	1.308(3)

References:

1. CrysAlisPro, Oxford Diffraction Ltd., version 1.171.33.49b, 2009.
2. L. J. Farrugia, WinGX, version 1.64, An Integrated System of Windows Programs for the Solution, Refinement and analysis of Single-Crystal X-ray Diffraction Data, Department of Chemistry, University of Glasgow, 2003.