Certificate of Analysis

Product Name: **CGP 60474** **Catalog No.: 5471** **Batch No.: 1**

CAS Number: 164658-13-3

IUPAC Name: 3-[[4-[2-[(3-Chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]amino]-1-propanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{18}ClN_5O.¼H_2O$

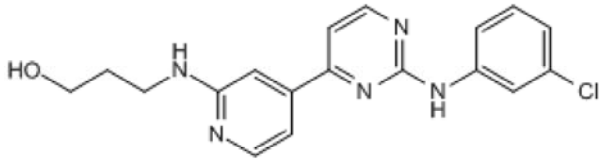
Batch Molecular Weight: 360.32

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
1eq. HCl to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.43 (Dichloromethane:Methanol:Ammonia soln. [89:10.1])

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60	5.17	19.44
Found	59.79	5.05	19.25

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Description:

Potent cyclin-dependent kinase (cdk) inhibitor (reported IC_{50} values are 3 - 80, 9.5, 13, 17 - 60, 200 and 220 nM for cdk2, cdk5, cdk9, cdk1, cdk4 and cdk7, respectively). Also inhibits PKCα in the low micromolar range. Displays reversible G1/S cell cycle arrest in U2-OS cells.

Physical and Chemical Properties:

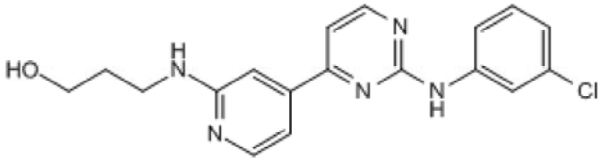
Batch Molecular Formula: $C_{18}H_{18}ClN_5O.¼H_2O$

Batch Molecular Weight: 360.32

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
1eq. HCl to 50 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Jorda *et al* (2018) How selective are pharmacological inhibitors of cell-cycle-regulating cyclin-dependent kinases? J.Med.Chem. ***61*** 9105. PMID: 30234987.

Stanetty *et al* (2005) Novel and efficient access to phenylamino-pyrimidine type protein kinase C inhibitors utilizing a Negishi cross-coupling strategy. J.Org.Chem. ***70*** 5215. PMID: 15960526.

Sielecki *et al* (2000) Cyclin-dependent kinase inhibitors: useful targets in cell cycle regulation. J.Med.Chem. ***43*** 1. PMID: 10633033.