

Product Name: Aminopurvalanol A

Catalog No.: 2072

Batch No.: 1

CAS Number: 220792-57-4

IUPAC Name: (2*R*)-2-[[6-[(3-Amino-5-chlorophenyl)amino]-9-(1-methylethyl)-9*H*-purin-2-yl]amino]-3-methyl-1-butanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₆ClN₇O.½H₂O

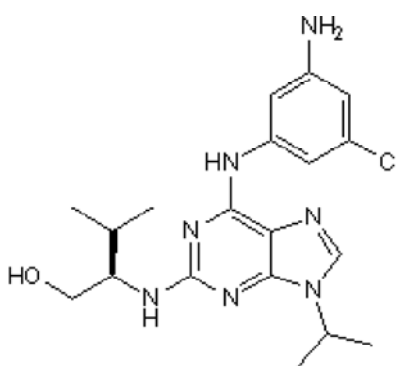
Batch Molecular Weight: 412.92

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.29 (Dichloromethane:Methanol [95:5])

Melting Point: Between 82 - 85°C

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

¹³C NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.27	6.59	23.74
Found	55.41	6.63	23.82

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Description:

Cyclin-dependent kinase (cdk) inhibitor (reported IC₅₀ values are 20 - 35 nM for cdk1, cdk2 and cdk5). Also inhibits ERK1 (IC₅₀ = 12.0 μM) and ERK2 (IC₅₀ = 3.1 μM) and is 3000-fold selective over a range of other protein kinases (IC₅₀ >100 μM). Arrests cell cycle at G2/M boundary (IC₅₀ = 1.25 μM), and induces apoptosis at concentrations >10 μM. Cell permeable.

Physical and Chemical Properties:

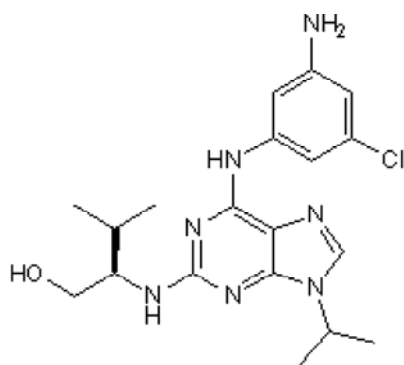
Batch Molecular Formula: C₁₉H₂₆ClN₇O·½H₂O

Batch Molecular Weight: 412.92

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 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.

Licensing Information:

Sold under license from the Regents of the University of California

References:

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

Knockaert et al (2000) Intracellular targets of cyclin-dependent kinase inhibitors: identification by affinity chromatography using immobilised inhibitors. *Chem.Biol.* **7** 411. PMID: 10873834.

Chang et al (1999) Synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors. *Chem.Biol.* **6** 361. PMID: 10375538.

Rosiana et al (1999) A cyclin-dependent kinase inhibitor inducing cancer cell differentiation: biochemical identification using *Xenopus* egg extracts. *Proc.Natl.Acad.Sci.USA* **96** 4797.

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