

Product Name: Purvalanol B

Catalog No.: 1581

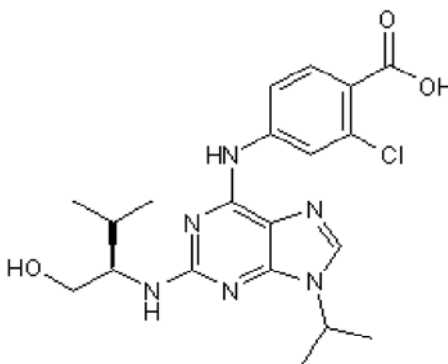
Batch No.: 7

CAS Number: 212844-54-7

IUPAC Name: (2*R*)-2-[[6-[(3-Chloro-4-carboxyphenyl)amino]-9*H*-purin-2-yl]amino]-3-methyl-1-butanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₅ClN₆O₃
Batch Molecular Weight: 432.91
Physical Appearance: White solid
Solubility: 1eq. NaOH to 100 mM with gentle warming
DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >99.1% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.49	5.82	19.41
Found	55.4	5.8	19.42

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Cyclin-dependent kinase (cdk) inhibitor (reported IC₅₀ values are 6 nM for cdk1 and cdk5, and 6 - 9 nM for cdk2, depending on binding partner). Selective over a range of other protein kinases (IC₅₀ >10,000 nM). Shown to have antiproliferative properties, mediated by ERK1 and ERK2.

Physical and Chemical Properties:

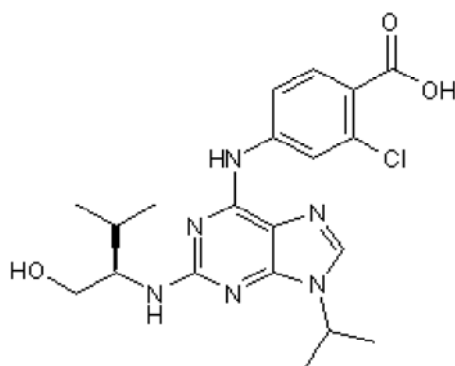
Batch Molecular Formula: C₂₀H₂₅ClN₆O₃

Batch Molecular Weight: 432.91

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

1eq. NaOH to 100 mM with gentle warming
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 (2002) p42/p44 MAPKs are intracellular targets of the CDK inhibitor purvalanol. *Oncogene* **21** 6413. PMID: 12226745.

Gray et al (1999) ATP-site directed inhibitors of cyclin-dependent kinases. *Curr.Med.Chem.* **6** 859. PMID: 10495356.

Gray et al (1998) Exploiting chemical libraries, structure, and genomics in the search for kinase inhibitors. *Science* **281** 533. PMID: 9677190.

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