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Print Date: May 4th 2022

Batch No.: 7

Certificate of Analysis

www.tocris.com

Catalog No.: 1581

Product Name: Purvalanol B

CAS Number: 212844-54-7

IUPAC Name:

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

1. PHYSICAL AND CHEMICAL PROPERTIES

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

Storage: Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis: Shows 98.9% purity Consistent with structure Consistent with structure 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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(2R)-2-[[6-[(3-Chloro-4-carboxyphenyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-1-butanol

Description:

Purvalanol B is a cyclin-dependent kinase (cdk) inhibitor (reported IC_{50} values are 6 nM for cdk1 and cdk5, and 6 - 9 nM for cdk2, depending on binding partner). Purvalanol B is selective over a range of other protein kinases (IC_{50} >10,000 nM). Purvalanol B shows antiproliferative properties, mediated by ERK1 and ERK2. Purvalanol B induces autophagy in cellular models and induces apoptosis in cancer cells, the apoptotic effects can be increased by combining with Rapamycin (Cat. No. 1292).

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:

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References:

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

Ozfiliz-Kilbas *et al* (2018) Cyclin-dependent kinase inhibitors, roscovitine and purvalanol, induce apoptosis and autophagy related to unfolded protein response in HeLa cervical cancer cells. Mol.Biol.Rep. **45** 815. PMID: 29978381.

Knockaert et al (2002) p42/p44 MAPKs are intracellular targets of the CDK inhibitor purvalanol. Oncogene 21 6413. PMID: 12226745.

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