

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: PCI 29732 Catalog No.: 5012 Batch No.: 1

CAS Number: 330786-25-9

IUPAC Name: 1-Cyclopentyl-3-(4-phenoxyphenyl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-4-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{21}N_5O$ Batch Molecular Weight:371.44Physical Appearance:Cream solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.3$ (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 71.14 5.7 18.85 Found 70.89 5.64 18.69



Product Information

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IUPAC Name: 1-Cyclopentyl-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine

Description:

Potent BTK inhibitor ($IC_{50} = 0.3$ nM). Blocks B cell antigen receptor (BCR)-mediated gene expression in CD20+ B cells.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₂H₂₁N₅O Batch Molecular Weight: 371.44 Physical Appearance: Cream solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Honigberg et al (2010) The Bruton tyrosine kinase inhibitor PCI-32765 blocks B-cell activation and is efficacious in models of autoimmune disease and B-cell malignancy. Proc.Natl.Acad.Sci.U.S.A. 107 13075. PMID: 20615965.

Krishnamurty et al (2013) Active site profiling reveals coupling between domains in SRC-family kinases. Nat. Chem. Biol. 9 43. PMID: 23143416.