

Certificate of Analysis

Print Date: Sep 26th 2022

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Product Name: AZ PFKFB3 26 Catalog No.: 5675 Batch No.: 1

CAS Number: 1704740-52-2

IUPAC Name: (2S)-N-[4-[[3-Cyano-1-(2-methylpropyl)-1*H*-indol-5-yl]oxy]phenyl]-2-pyrrolidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{26}N_4O_2$ Batch Molecular Weight:402.49Physical Appearance:White solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.19$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 71.62 6.51 13.92 Found 71.94 6.56 13.8

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

5 529449 www.tocris.com/distributors Tel:+1 612 379 2956



Product Information

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IUPAC Name: (2S)-N-[4-[[3-Cyano-1-(2-methylpropyl)-1*H*-indol-5-yl]oxy]phenyl]-2-pyrrolidinecarboxamide

Description:

AZ PFKFB3 26 is a potent and selective PFKFB3 inhibitor (IC $_{50}$ = 0.023 μ M). Selective for PFKFB3 over PFKFB2 and PFKFB1 isoforms (IC $_{50}$ values are 0.382 μ M and 2.06 μ M, respectively). Reduces levels of fructose-1,6-bisphosphate in A549 cells (IC $_{50}$ = 0.343 μ M). Exhibits no significant inhibition of other kinases.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{24}H_{26}N_4O_2$ Batch Molecular Weight: 402.49 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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.

References:

Boyd *et al* (2015) Structure-based design of potent and selective inhibitors of the metabolic kinase PFKFB3. J.Med.Chem. **58** 3611. PMID: 25849762.

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