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Print Date: Oct 15th 2016

Certificate of Analysis

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Product Name: **AZ PFKFB3 67** **Catalog No.: 5742** **Batch No.: 1**

CAS Number: 1704741-11-6

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{25}N_5O_3 \cdot ¼H_2O$

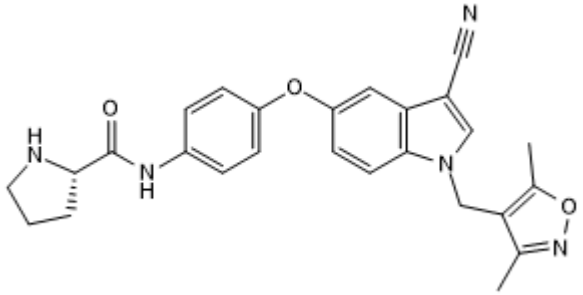
Batch Molecular Weight: 460.01

Physical 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

Chiral HPLC: Shows >99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -35.1 (Concentration = 1, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.88	5.59	15.22
Found	67.69	5.45	15.11

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

Potent and selective PFKFB3 inhibitor (IC_{50} values are 11, 159 and 1130 nM for PFKFB3, PFKFB2 and PFKFB1 respectively).

Physical and Chemical Properties:

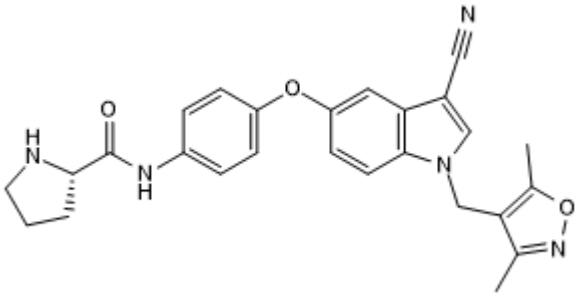
Batch Molecular Formula: $C_{26}H_{25}N_5O_3.¼H_2O$

Batch Molecular Weight: 460.01

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.

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
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Tel:+1 612 379 2956