# biotechne<sup>®</sup> TOCRIS

IUPAC Name:

# Certificate of Analysis

# www.tocris.com

Batch No.: 3

Catalog No.: 5742

Print Date: May 16th 2024

### Product Name: AZ PFKFB3 67

CAS Number: 1704741-11-6

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>26</sub>H<sub>25</sub>N<sub>5</sub>O<sub>3</sub>. 455.51 White solid DMSO to 100 mM ethanol to 100 mM Store at -20°C

Storage: Batch Molecular Structure:

N

### 2. ANALYTICAL DATA

HPLC: Chiral HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 98.8% purity Shows 99.0% purity Consistent with structure Consistent with structure

|             | Carbon Hydrogen Nitrog |      |       |  |  |
|-------------|------------------------|------|-------|--|--|
| Theoretical | 68.56                  | 5.53 | 15.37 |  |  |
| Found       | 67.67                  | 5.6  | 15.01 |  |  |

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

| bio-techne.com                                    | North America       | China  | Europe Middle East Africa | Rest of World                                      |
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(2S)-N-[4-[[3-Cyano-1-[(3,5-dimethyl-4-isoxazolyl)methyl]-1H-indol-5-yl]oxy]phenyl]-2-pyrrolidinecarboxamide

#### Description:

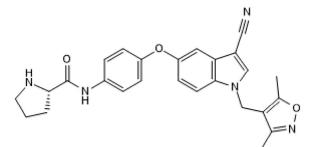
AZ PFKFB3 67 is a potent and selective PFKFB3 inhibitor (IC<sub>50</sub> values are 11, 159 and 1130 nM for PFKFB3, PFKFB2 and PFKFB1 respectively).

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>26</sub>H<sub>25</sub>N<sub>5</sub>O<sub>3</sub>. Batch Molecular Weight: 455.51 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  $45-60^{\circ}C$  water bath).

Catalog No.: 5742

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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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