Certificate of Analysis

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BI 78D3 Product Name:

Catalog No.: 3314

Batch No.: 1

Print Date: Jul 1st 2019

CAS Number: IUPAC Name:

Storage:

883065-90-5

4-(2,3-Dihydro-1,4-benzodioxin-6-yl)-2,4-dihydro-5-[(5-nitro-2-thiazolyl)thio]-3H-1,2,4-triazol-3-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

 $C_{13}H_9N_5O_5S_2$ 379.37 Beige solid DMSO to 100 mM ethanol to 5 mM

Batch Molecular Structure:

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s _ s	
O2N	

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 99.3% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen			
Theoretical	41.16	2.39	18.46	
Found	41.21	2.41	18.38	

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

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Store at +4°C _

TOCRIS a biotechne brand

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Product Name: BI 78D3

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4-(2,3-Dihydro-1,4-benzodioxin-6-yl)-2,4-dihydro-5-[(5-nitro-2-thiazolyl)thio]-3H-1,2,4-triazol-3-one

Description:

IUPAC Name:

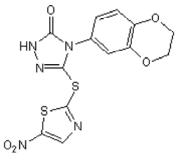
Competitive c-Jun N-terminal kinase (JNK) inhibitor (IC₅₀ = 280 nM) that displays > 100 fold selectivity over p38 α and no activity at mTOR and PI-3K. Inhibits JNK interacting protein 1 (JIP1) -JNK binding (IC₅₀ = 500 nM) and prevents JNK substrate phosphorylation. Blocks JNK-dependent Con A-induced liver damage and restores insulin sensitivity in a mouse model of type II diabetes.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{13}H_9N_5O_5S_2$ Batch Molecular Weight: 379.37 Physical Appearance: Beige solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Flight (2008) Getting rid of JNK. Nat.Rev.Drug Disc. 7 975.
Haas and Writer (2008) Block JNK at the dock. SCiBX 1.
Stebbins *et al* (2008) Identification of a new JNK inhibitor targeting the JNK-JIP interaction site. Proc.Natl.Acad.Sci.USA 105 16809.

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Storage: Store at +4°C

Solubility & Usage Info: DMSO to 100 mM ethanol to 5 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.: 3314

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.