

**Product Name:** BI 78D3

**Catalog No.:** 3314

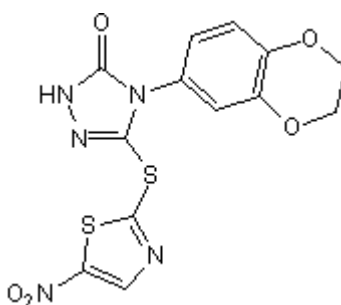
**Batch No.:** 1

**CAS Number:** 883065-90-5

**IUPAC Name:** 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:** C<sub>13</sub>H<sub>9</sub>N<sub>5</sub>O<sub>5</sub>S<sub>2</sub>  
**Batch Molecular Weight:** 379.37  
**Physical Appearance:** beige solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 5 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows >99.3% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	41.16	2.39	18.46
Found	41.21	2.41	18.38

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**Description:**

Competitive c-Jun N-terminal kinase (JNK) inhibitor ( $IC_{50}$  = 280 nM) that displays > 100 fold selectivity over p38 $\alpha$  and no activity at mTOR and PI-3K. Inhibits JNK interacting protein 1 (JIP1)-JNK binding ( $IC_{50}$  = 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:**

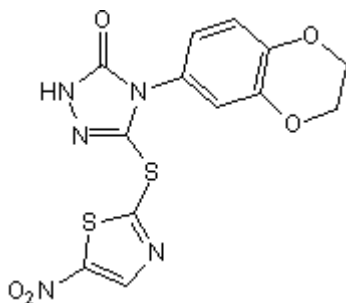
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Batch Molecular Weight: 379.37

Physical Appearance: beige solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Stebbins *et al*** (2008) Identification of a new JNK inhibitor targeting the JNK-JIP interaction site. *Proc.Natl.Acad.Sci.USA* **105** 16809.

**Flight** (2008) Getting rid of JNK. *Nat.Rev.Drug Disc.* **7** 975.

**Haas and Writer** (2008) Block JNK at the dock. *SCiBX* **1** 1.

**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°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.

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