

# **Certificate of Analysis**

Print Date: Dec 9th 2020

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Product Name: TCS JNK 5a Catalog No.: 2827 Batch No.: 2

CAS Number: 312917-14-9

IUPAC Name: N-(3-Cyano-4,5,6,7-tetrahydrobenzo[b]thienyl-2-yl)-1-naphthalenecarboxamide

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{20}H_{16}N_2OS.\frac{1}{4}H_2O$ 

Batch Molecular Weight: 336.92

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 99.5% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 71.3 4.94 8.31 Found 71.65 4.87 8.4



## **Product Information**

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IUPAC Name: N-(3-Cyano-4,5,6,7-tetrahydrobenzo[b]thienyl-2-yl)-1-naphthalenecarboxamide

#### **Description:**

Selective inhibitor of JNK2 and JNK3 (pIC $_{50}$  values are 6.7, 6.5, <5.0 and <4.8 for JNK3, JNK2, JNK1 and p38 $\alpha$  respectively). Displays no significant activity at a range of other protein kinases including EGFR, ErbB2, cdk2, PLK-1 and Src (pIC $_{50}$  < 5.0).

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>OS.1/4H<sub>2</sub>O

Batch Molecular Weight: 336.92 Physical Appearance: White solid

Minimum Purity: ≥99%

#### **Batch Molecular Structure:**

Storage: Store at RT

#### Solubility & Usage Info:

DMSO 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:

**Angell** *et al* (2007) *N*-(3-cyano-4,5,6,7-tetrahydro-1-benzothien-2-yl)amides as potent, selective, inhibitors of JNK2 and JNK3. Bioorg.Med.Chem.Letts. *17* 1296.

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