

**Certificate of Analysis** 

Print Date: Jan 16th 2016

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Product Name: BTB1 Catalog No.: 5399 Batch No.: 1

CAS Number: 86030-08-2

IUPAC Name: 4-Chloro-2-nitro-1-(phenylsulfonyl)benzene

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C<sub>12</sub>H<sub>8</sub>CINO<sub>4</sub>S

Batch Molecular Weight: 297.71

Physical Appearance: White solid

**Solubility:** DMSO to 100 mM

ethanol to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:

# 2. ANALYTICAL DATA

Melting Point:Between 117 - 119°CHPLC:Shows 99.6% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 48.41 2.71 4.7 Found 48.48 2.68 4.68



# **Product Information**

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# **Description:**

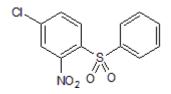
Selective and ATP-competitive mitotic kinesin Kif18A inhibitor (IC $_{50}$  = 1.7  $\mu$ M); reversibly inhibits microtubule-stimulated Kif18A ATPase activity. Displays selectivity against a panel of other mitotic kinesins.

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

Batch Molecular Formula: C<sub>12</sub>H<sub>8</sub>CINO<sub>4</sub>S Batch Molecular Weight: 297.71 Physical Appearance: White solid

Minimum Purity: >99%

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



Storage: Store at +4°C

# Solubility & Usage Info:

DMSO to 100 mM ethanol to 20 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:

Catarinella et al (2009) BTB-1: a small molecule inhibitor of the mitotic motor protein Kif18A. Angew.Chem.Int.Ed.Engl. 48 9072. PMID: 19856362.

**Braun** et al (2014) Synthesis and biological evaluation of optimized Inhibitors of the mitotic kinesin Kif18A. ACS Chem.Biol. 10 554. PMID: 25402598.

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