

# **Certificate of Analysis**

Print Date: Jan 14th 2016

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Product Name: TC Mps1 12 Catalog No.: 4750 Batch No.: 1

CAS Number: 1206170-62-8

IUPAC Name: 4-[[4-Amino-5-cyano-6-[(1,1-dimethylethyl)amino]-2-pyridinyl]amino]benzamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{17}H_{20}N_6O.14H_2O$ 

**Batch Molecular Weight:** 328.88 **Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

ethanol to 20 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.43$  (Ethyl acetate)

HPLC: Shows 100% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 62.08 6.28 25.55 Found 62.4 6.24 25.27



# **Product Information**

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# **Description:**

Potent and selective monopolar spindle 1 (Mps1) inhibitor ( $IC_{50}$  = 6.4 nM). Selective for Mps1 over a panel of 95 kinases including JNK. Inhibits A549 lung carcinoma cell proliferation and attenuates A549 cell xenograft growth in mice. Orally active.

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

Batch Molecular Formula: C<sub>17</sub>H<sub>20</sub>N<sub>6</sub>O.1/4H<sub>2</sub>O

Batch Molecular Weight: 328.88 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 with gentle warming

#### 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:

Kusakabe et al (2012) Diaminopyridine-based potent and selective mps1 kinase inhibitors binding to an unusual flipped-Peptide conformation. ACS Med.Chem.Lett. 3 560. PMID: 24900510.