

# **Certificate of Analysis**

Print Date: Jan 14th 2016

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Product Name: CCT 137690 Catalog No.: 4291 Batch No.: 2

CAS Number: 1095382-05-0

IUPAC Name: 6-Bromo-7-[4-[(5-methyl-3-isoxazolyl)methyl]-1-piperazinyl]-2-[4-(4-methyl-1-piperazinyl)phenyl]-3*H*-imidazo[4,5-*b*]

pyridine

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{26}H_{31}BrN_8O$ 

**Batch Molecular Weight:** 551.48 **Physical Appearance:** Yellow solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.19$  (Chloroform:Methanol:Ammonia soln. [9:1:0.1])

HPLC: Shows 99.1% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 56.63 5.67 20.32 Found 56.5 5.68 20.24



## **Product Information**

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pyridine

#### **Description:**

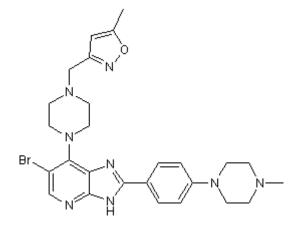
Potent inhibitor of Aurora kinases (IC<sub>50</sub> values are 0.015, 0.019 and 0.025 µM at Aurora A, Aurora C and Aurora B respectively). Displays antiproliferative activity in a range of human tumor cell lines. Orally bioavailable.

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

Batch Molecular Formula: C<sub>26</sub>H<sub>31</sub>BrN<sub>8</sub>O Batch Molecular Weight: 551.48 Physical Appearance: Yellow solid

Minimum Purity: >98%

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



Storage: Store at +4°C

### 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:

Bavetsias et al (2010) Imidazo[4,5-b]pyridine derivatives as inhibitors of Aurora kinases: lead optimization studies toward the identification of an orally bioavailable preclinical development candidate. J.Med.Chem. 53 5213. PMID: 20565112.

Faisal et al (2011) The Aurora kinase inhibitor CCT137690 downregulates MYCN and sensitizes MYCN-amplified neuroblastoma in vivo. Mol.Cancer Ther. 10 2115. PMID: 21885865.

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