

**Certificate of Analysis** 

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Print Date: Jan 16th 2016

Product Name: KG 5 Catalog No.: 5260 Batch No.: 1

CAS Number: 877874-85-6

IUPAC Name: 2-(Methylthio)-6-[4-[5-[[3-(trifluoromethyl)phenyl]amino]-1<sub>H</sub>-1,2,4-triazol-3-yl]phenoxy]-4-pyrimidinamine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{20}H_{16}F_3N_7OS.H_2O$ 

Batch Molecular Weight: 477.47

Physical Appearance: White solid

**Solubility:** DMSO to 100 mM ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:** 

F<sub>3</sub>C N-N NH<sub>2</sub>

# 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.3 \text{ (DCM/MeOH/NH4OH 9/1/5 drops)}$ 

HPLC: Shows 99.7% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 50.31 3.8 20.53 Found 50.34 3.51 20.4



# **Product Information**

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### **Description:**

PDGFRβ and B-Raf allosteric inhibitor. Also inhibits c-Raf, FLT3 and KIT. Disrupts blood vessel formation in zebrafish embryos and inhibits angiogenesis in a mouse angiogenesis model. Inhibits growth of renal and pancreatic tumors in mice. Also arrests cells in prometaphase. Orally available.

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

Batch Molecular Formula: C<sub>20</sub>H<sub>16</sub>F<sub>3</sub>N<sub>7</sub>OS.H<sub>2</sub>O

Batch Molecular Weight: 477.47 Physical Appearance: White solid

Minimum Purity: >98%

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

**Storage:** Store at -20°C

# Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Murphy et al (2010) Disruption of angiogenesis and tumor growth with an orally active drug that stabilizes the inactive state of PDGFRbeta/B-RAF. Proc.Natl.Acad.Sci.U.S.A. 107 4299. PMID: 20154271.

Mielgo et al (2011) A MEK-independent role for CRAF in mitosis and tumor progression. Nat.Med. 17 (1641). PMID: 22081024.