

# **Certificate of Analysis**

Print Date: Oct 30th 2018

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**Product Name:** LY 364947 Catalog No.: 2718 Batch No.: 1

CAS Number: 396129-53-6

**IUPAC Name:** 4-[3-(2-Pyridinyl)-1H-pyrazol-4-yl]-quinoline

## 1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{17}H_{12}N_4$ **Batch Molecular Formula: Batch Molecular Weight:** 272.31 **Physical Appearance:** Tan solid

DMSO to 100 mM Solubility:

Storage: Store at RT

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

TLC:  $R_f = 0.2$  (Chloroform:Methanol [8:2])

**Melting Point:** Between 241 - 242°C **HPLC**: Shows >99.6% purity <sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 74.98 4.44 20.56 Found 74.64 4.43 20.48

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# **Product Information**

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#### **Description:**

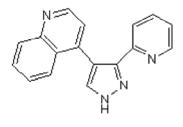
Selective inhibitor of TGF- $\beta$  type-I receptor (TGF- $\beta$  RI, TGFR-I, T $\beta$ R-I, ALK-5) (IC $_{50}$  values are 59, 400 and 1400 nM for TGR- $\beta$  RI, TGF- $\beta$  RII and MLK-7K respectively). Inhibits TGF- $\beta$ -dependent luciferase production in mink lung cells (p3TP lux) and growth in mouse fibroblasts (NIH 3T3) (IC $_{50}$  values are 47 and 89 nM respectively). Suppresses invasion of MDA-MB-231 breast cancer cells in a matrigel invasion assay.

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

Batch Molecular Formula: C<sub>17</sub>H<sub>12</sub>N<sub>4</sub> Batch Molecular Weight: 272.31 Physical Appearance: Tan solid

**Minimum Purity:** >99%

# **Batch Molecular Structure:**



Storage: Store at RT

## Solubility & Usage Info:

DMSO to 100 mM

When purched as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

# 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:

**Li** *et al* (2006) Dihydropyrrolopyrazole transforming growth factor-β type I receptor kinase domain inhibitors: a novel benzimidazole series with selectivity versus transforming growth factor-β type II receptor kinase and mixed lineage kinase 7. J.Med.Chem. *49* 2138. PMID: 16539403.

**Shiou** *et al* (2006) Smad4-dependent regulation of urokinase plasminogen activator secretion and RNA stability associated with invasiveness by autocrine and paracrine transforming growth factor-β. J.Biol.Chem. *281* 33971. PMID: 16959768.

**Sawyer** *et al* (2003) Synthesis and activity of new aryl- and heteroaryl-substituted pyrazole inhibitors of the transforming growth factor-µ type I receptor kinase domain. J.Med.Chem. *46* 3953. PMID: 12954047.