

# **Certificate of Analysis**

Print Date: May 3<sup>rd</sup> 2017

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Product Name: LDN 212854 Catalog No.: 6151 Batch No.: 1

CAS Number: 1432597-26-6

IUPAC Name: 5-(6-(4-(1-Piperazinyl)phenyl)pyrazolo[1,5-a]pyrimidin-3-yl)quinoline

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{25}H_{22}N_6.1\frac{1}{4}H_2O$ 

Batch Molecular Weight: 429

Physical Appearance: Yellow solid

**Solubility:** 2eq.HCl to 50 mM

DMSO to 3 mM with gentle warming

Storage: Store at -20°C

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**HPLC:** Shows 98.7% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 69.99 5.76 19.59 Found 70.2 5.51 19.62



# **Product Information**

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IUPAC Name: 5-(6-(4-(1-Piperazinyl)phenyl)pyrazolo[1,5-a]pyrimidin-3-yl)quinoline

#### **Description:**

Potent ALK inhibitor (IC $_{50}$  values are 1.3, 2.4, 85.8, 2,133 and 9,276 nM for ALK2, ALK1, ALK3, ALK4 and ALK5, respectively). Exhibits selectivity for ALK2 over ALK4 and ALK5 in cellular assays. Inhibits heterotopic ossification in a mutant ALK2 mouse model of fibrodysplasia ossificans progressiva. Also exhibits activity against RIPK2, ABL1 and PDGFR- $\beta$  (IC $_{50}$  values < 100 nM).

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

Batch Molecular Formula: C<sub>25</sub>H<sub>22</sub>N<sub>6</sub>.11/4H<sub>2</sub>O

Batch Molecular Weight: 429 Physical Appearance: Yellow solid

Minimum Purity: >98%

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

Storage: Store at -20°C

#### Solubility & Usage Info:

2eq.HCl to 50 mM

DMSO to 3 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.

# **Licensing Information:**

Sold for research purposes under exclusive agreement from The Brigham and Women's Hospital Inc. US patent 14/776,302

References:

Mohedas et al (2013) Development of an ALK2-biased BMP type I receptor kinase inhibitor. ACS Chem.Biol. 8 1291. PMID: 23547776.