

Certificate of Analysis

Print Date: May 3rd 2017

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Product Name: LDN 214117 Catalog No.: 6152 Batch No.: 1

CAS Number: 1627503-67-6

IUPAC Name: 1-[4-[6-Methyl-5-(3,4,5-trimethoxyphenyl)-3-pyridinyl]phenyl]piperazine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{29}N_3O_3$ Batch Molecular Weight: 419.52

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

HN O O

2. ANALYTICAL DATA

HPLC: Shows 99% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 71.57 6.97 10.02 Found 71.57 6.95 10.04



Product Information

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IUPAC Name: 1-[4-[6-Methyl-5-(3,4,5-trimethoxyphenyl)-3-pyridinyl]phenyl]piperazine

Description:

Potent and selective inhibitor of type I bone morphogenic protein (BMP) receptor ALK2 (IC_{50} = 24 nM). Shows preference for ALK1 and ALK2 over ALK3 and 164-fold selectivity for BMP6 inhibition (IC $_{50}$ = 100 nM) over TGF- β 1. Exhibits improved kinome selectivity over K 02288 (Cat.No. 4986) and low cytotoxicity.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₅H₂₉N₃O₃ Batch Molecular Weight: 419.52 Physical Appearance: Off 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.

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 (2014) Structure-activity relationship of 3,5-diaryl-2-aminopyridine ALK2 inhibitors reveals unaltered binding affinity for fibrodysplasia ossificans progressiva causing mutants. J Med Chem. 57 7900. PMID: 25101911.