

Certificate of Analysis

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Print Date: Jan 14th 2016

Product Name: K 02288 Catalog No.: 4986 Batch No.: 1

CAS Number: 1431985-92-0

IUPAC Name: 3-[(6-Amino-5-(3,4,5-trimethoxyphenyl)-3-pyridinyl]phenol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{20}N_2O_4.4H_2O$

Batch Molecular Weight: 356.88

Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM

ethanol to 10 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

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

Microanalysis: Carbon Hydrogon Nitrogo

Carbon Hydrogen Nitrogen

Theoretical 67.31 5.79 7.85 Found 67.62 5.62 7.94



Product Information

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IUPAC Name: 3-[(6-Amino-5-(3,4,5-trimethoxyphenyl)-3-pyridinyl]phenol

Description:

Potent and selective inhibitor of type I bone morphogenic protein (BMP) receptors (IC $_{50}$ values are 1.1, 1.8, 6.4, 34.4, 220, 302 and 321 nM for ALK2, ALK1, ALK6, ALK3, ActRIIA, ALK4 and ALK5 respectively). Reduces BMP4-induced Smad1/5/8 phosphorylation in vitro ($IC_{50} = 100$ nM) and induces dorsalization of zebrafish embryos.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₂₀N₂O₄. ¼ H₂O

Batch Molecular Weight: 356.88 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 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.

References:

Sanvitale et al (2013) A new class of small molecule inhibitor of BMP signaling. PLoS ONE 8 62721. PMID: 23646137.

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