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Certificate of Analysis

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Product Name: BI 9564

Catalog No.: 5590 Batch No.: 1

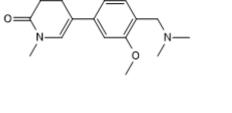
CAS Number: IUPAC Name: 1883429-22-8

4-[4-[(Dimethylamino)methyl]-2,5-dimethoxyphenyl]-2-methyl-1,2-dihydro-2,7-naphthyridin-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₂₀H₂₃N₃O₃.¹/₄H₂O 357.91 Brown solid DMSO to 20 mM 1eq. HCl to 10 mM with gentle warming ethanol to 20 mM Store at -20°C

Storage: Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: R_f = 0.4 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1]) Shows 98.6% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen

Theoretical	67.11	6.62	11.74
Found	67.05	6.48	11.56

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Print Date: Jun 23rd 2016

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CAS Number:

4-[4-[(Dimethylamino)methyl]-2,5-dimethoxyphenyl]-2-methyl-1,2-dihydro-2,7-naphthyridin-1-one

Description:

IUPAC Name:

Potent and selective BRD9 and BRD7 inhibitor (K_d values are 14 and 239 nM, respectively). Exhibits selectivity for BRD9/7 over 48 other bromodomains, 324 kinases and 55 GPCRs. Inhibits proliferation of AML cell lines in vitro and reduces AML tumor xenograft growth in vivo. Orally active.

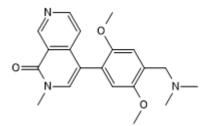
1883429-22-8

Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₂₃N₃O₃. ¼H₂O Batch Molecular Weight: 357.91 Physical Appearance: Brown solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM 1eq. HCl to 10 mM with gentle warming ethanol to 20 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).

Catalog No.: 5590

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:

Martin et al (2016) Structure-based design of an in vivo active selective BRD9 inhibitor J.Med.Chem. 59 4462. PMID: 26914985.

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