



Certificate of Analysis

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Product Name: UNC 1999 Catalog No.: 4904 Batch No.: 1

CAS Number: 1431612-23-5

IUPAC Name: N-[(1,2-Dihydro-6-methyl-2-oxo-4-propyl-3-pyridinyl)methyl]-1-(1-methylethyl)-6-[6-[4-(1-methylethyl)-1-piperazinyl]-

3-pyridinyl]-1*H*-indazole-4-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{33}H_{43}N_7O_2$. $\frac{1}{2}H_2O$

Batch Molecular Weight: 578.75 **Physical Appearance:** White solid

Solubility: 1eq. HCl to 100 mM

DMSO to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.2$ (Dichloromethane:Methanol [19:1])

HPLC: Shows 99.6% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 68.49 7.66 16.94 Found 68.7 7.61 17.05



Product Information

Print Date: Apr 28th 2015

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3-pyridinyl]-1*H*-indazole-4-carboxamide

Description:

Potent and SAM-competitive EZH2/EZH1 lysine methyltransferase inhibitor (IC $_{50}$ values are 2 and 45 nM respectively). Selective for EZH2/EZH1 over a panel of other methyltransferases and non-epigenetic targets. Reduces H3K27me3 levels in vitro. Prolongs survival of MLL-AF9 bearing mice. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₃H₄₃N₇O₂.½H₂O

Batch Molecular Weight: 578.75 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

1eq. HCl to 100 mM DMSO 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).

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:

Konze *et al* (2013) An orally bioavailable chemical probe of the Lysine Methyltransferases EZH2 and EZH1. ACS Chem.Biol. *8* 1324. PMID: 23614352.

Xu et al (2015) Selective inhibition of EZH2 and EZH1 enzymatic activity by a small molecule suppresses MLL-rearranged leukemia. Blood 125 346. PMID: 25395428.

