

# **Certificate of Analysis**

Print Date: Dec 14th 2017

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**Product Name: UNC 2400** Catalog No.: 4905 Batch No.: 2

1433200-49-7 CAS Number:

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

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

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>35</sub>H<sub>47</sub>N<sub>7</sub>O<sub>2</sub>.½H<sub>2</sub>O

**Batch Molecular Weight:** 606.8

**Physical Appearance:** Off White solid Solubility: DMSO to 100 mM

1eq. HCl to 100 mM

Store at +4°C Storage:

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

Microanalysis:

TLC:  $R_f = 0.25$  (Dichloromethane:Methanol [95:5])

HPLC: Shows >99.2% purity <sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 69.28 7.97 16.16 Found 69.28 7.92 15.92

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

Tel:+1 612 379 2956



## **Product Information**

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

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

#### **Description:**

Negative control of UNC 1999. Exhibits 1000-fold lower potency than active analog ( $IC_{50}$  values are 62 and >200  $\mu$ M for EZH1 and EZH2, respectively). Active Analog also available.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>35</sub>H<sub>47</sub>N<sub>7</sub>O<sub>2</sub>.½H<sub>2</sub>O

Batch Molecular Weight: 606.8 Physical Appearance: Off White solid

**Minimum Purity:** >98%

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

**Storage:** Store at +4°C

## Solubility & Usage Info:

DMSO to 100 mM 1eq. HCl 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:**

This compound is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the UNC 1999 probe summary on the SGC website.

## References:

**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.

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

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