

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: C₃₃H₄₃N₇O₂·½H₂O

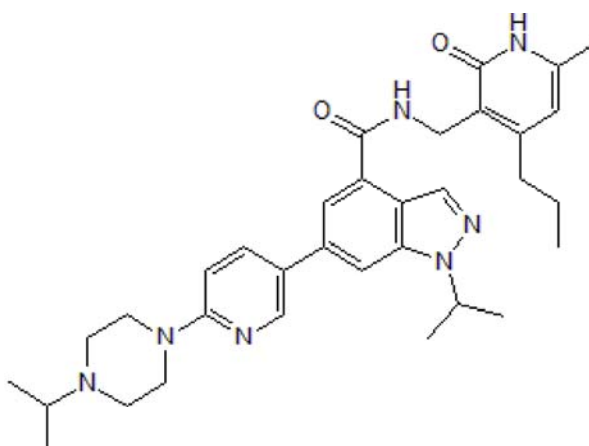
Batch Molecular Weight: 578.75

Physical Appearance: White solid

Solubility: 1M 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

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

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Description:

Potent and SAM-competitive EZH2/EZH1 lysine methyltransferase inhibitor (IC₅₀ values are 10 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. Negative Control also available.

Physical and Chemical Properties:

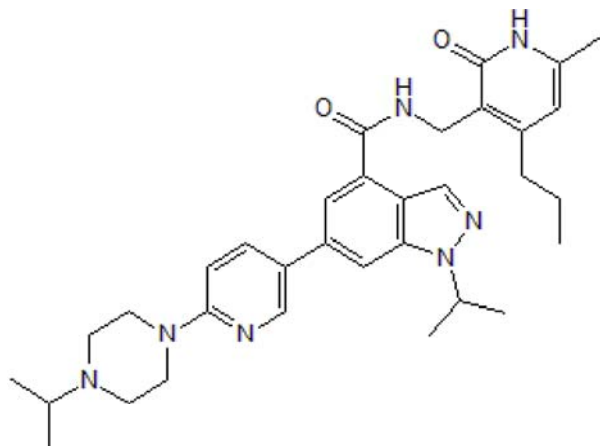
Batch Molecular Formula: C₃₃H₄₃N₇O₂·½H₂O

Batch Molecular Weight: 578.75

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

1M 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.

Licensing Information:

This probe 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:

Scheer et al (2019) A chemical biology toolbox to study protein methyltransferases and epigenetic signaling. *Nat.Commun.* **10** 19. PMID: 30604761.

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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