Print Date: Mar 3rd 2023

Certificate of Analysis

www.tocris.com

Product Name: **3-Deazaneplanocin A hydrochloride** **Catalog No.: 4703** **Batch No.: 8**

CAS Number: 120964-45-6

IUPAC Name: (1*S*,2*R*,5*R*)-5-(4-Amino-1*H*-imidazo[4,5-*c*]pyridin-1-yl)-3-(hydroxymethyl)-3-cyclopentene-1,2-diol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{14}N_4O_3.HCl.H_2O$

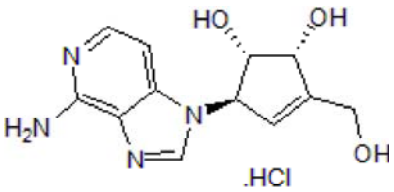
Batch Molecular Weight: 316.75

Physical Appearance: Beige solid

Solubility: water to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -111.7 (Concentration = 0.106, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	45.5	5.41	17.69
Found	44.98	5.13	17.29

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Description:

3-Deazaneplanocin A hydrochloride is a histone methyltransferase inhibitor; decreases global histone methylation. 3-Deazaneplanocin A hydrochloride inhibits EZH2 histone methyltransferase and s-adenosylhomocysteine (SAH) hydrolase activity. Blocks trimethylation of lysine 27 on histone H3 and lysine 20 on histone H4 in vitro. 3-Deazaneplanocin A hydrochloride induces apoptosis in multiple cancer cell lines and has no apoptotic effect on normal cells. Enhances Oct4 expression in chemically induced pluripotent stem cells (CiPSCs). DZNep synthesized to Ancillary Material Grade also available. For more information about how 3-Deazaneplanoc... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

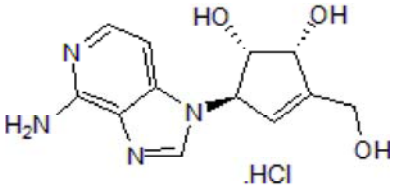
Batch Molecular Formula: $C_{12}H_{14}N_4O_3.HCl.H_2O$

Batch Molecular Weight: 316.75

Physical Appearance: Beige solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 10 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Hou *et al* (2013) Pluripotent stem cells induced from mouse somatic cells by small-molecule compounds. Science ***341*** 651. PMID: 23868920.

Miranda *et al* (2009) DZNep is a global histone methylation inhibitor that reactivates developmental genes not silenced by DNA methylation. Mol.Cancer Ther. ***8*** 1579. PMID: 19509260.

Tan *et al* (2007) Pharmacologic disruption of Polycomb-repressive complex 2-mediated gene repression selectively induces apoptosis in cancer cells. Genes Dev. ***21*** 1050. PMID: 17437993.