Print Date: May 30th 2012

Certificate of Analysis

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Product Name: UNC 0646 **Catalog No.: 4342** **Batch No.: 1**

CAS Number: 1320288-17-2

IUPAC Name: *N*-(1-Cyclohexyl-4-piperidinyl)-2-[hexahydro-4-(1-methylethyl)-1*H*-1,4-diazepin-1-yl]-6-methoxy-7-[3-(1-piperidinyl)propoxy]-4-quinazolinamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{36}H_{59}N_7O_2.{}^{3}/_{4}H_2O$

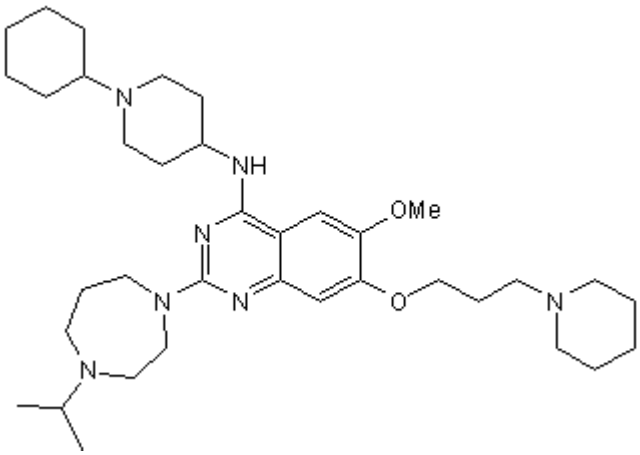
Batch Molecular Weight: 635.41

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.32 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.05	9.6	15.43
Found	67.75	9.51	15.35

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Description:

Potent and selective inhibitor of the homologous protein lysine methyltransferases, G9a and GLP (IC_{50} values are 6 nM and 15 nM for G9a and GLP, respectively). Potently blocks G9a/GLP methyltransferase activity in cells (IC_{50} = 10 nM in MCF7 cells); exhibits low cellular toxicity (EC_{50} = 4.7 µM in MCF7 cells). Selective for G9a/GLP over a range of other protein lysine methyltransferases and protein arginine methyltransferases.

Physical and Chemical Properties:

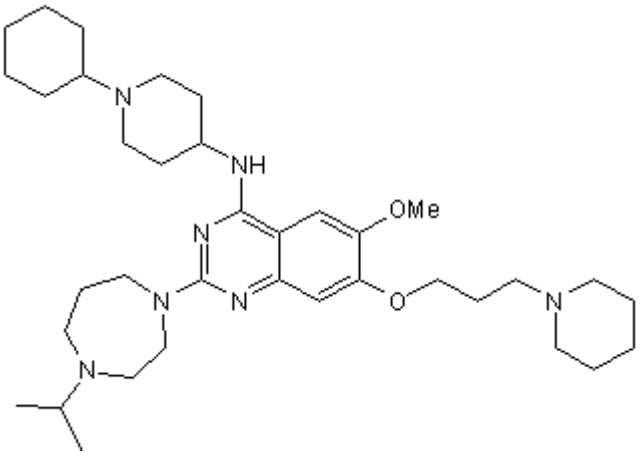
Batch Molecular Formula: $C_{36}H_{59}N_7O_2.¾H_2O$

Batch Molecular Weight: 635.41

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

References:

Liu *et al* (2011) Optimization of cellular activity of G9a inhibitors 7-aminoalkoxy-quinazolines. J.Med.Chem. ***54*** 6139. PMID: 21780790.