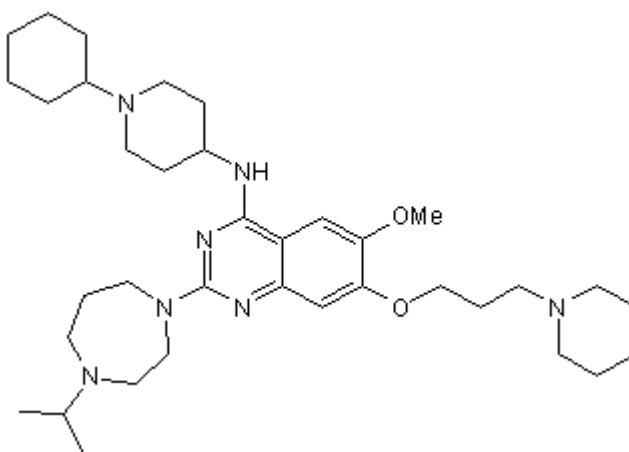


**Product Name:** UNC 0646 **Catalog No.:** 4342 **Batch No.:** 1  
**CAS Number:** 1320288-17-2  
**IUPAC Name:** *N*-(1-Cyclohexyl-4-piperidiny)-2-[hexahydro-4-(1-methylethyl)-1*H*-1,4-diazepin-1-yl]-6-methoxy-7-[3-(1-piperidiny)propoxy]-4-quinazolinamine

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>36</sub>H<sub>59</sub>N<sub>7</sub>O<sub>2</sub>·<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O  
**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<sub>f</sub> = 0.32 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])  
**HPLC:** Shows 99.4% purity  
**<sup>1</sup>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<sub>50</sub> values are 6 nM and 15 nM for G9a and GLP, respectively). Potently blocks G9a/GLP methyltransferase activity in cells (IC<sub>50</sub> = 10 nM in MCF7 cells); exhibits low cellular toxicity (EC<sub>50</sub> = 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:**

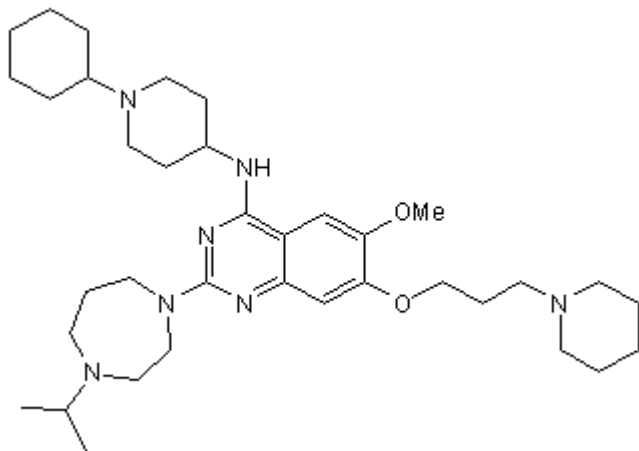
Batch Molecular Formula: C<sub>36</sub>H<sub>59</sub>N<sub>7</sub>O<sub>2</sub>·¾H<sub>2</sub>O

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.

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