

**Product Name:** UNC 0642

**Catalog No.:** 5132

**Batch No.:** 1

**CAS Number:** 1481677-78-4

**IUPAC Name:** 2-(4,4-Difluoro-1-piperidiny)-6-methoxy-*N*-[1-(1-methylethyl)-4-piperidiny]-7-[3-(1-pyrrolidinyl)propoxy]-4-quinazolinamine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{29}H_{44}F_2N_6O_2 \cdot \frac{1}{2}H_2O$

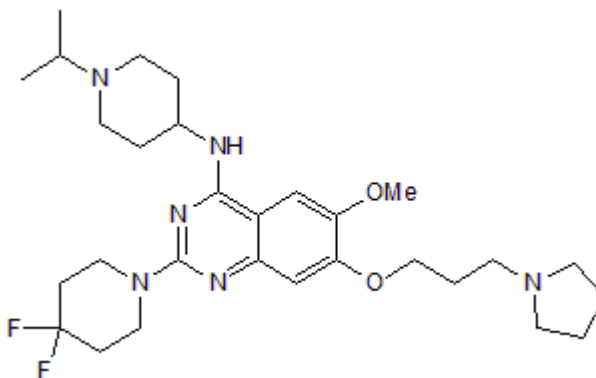
**Batch Molecular Weight:** 555.71

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
1eq. HCl to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.4$  (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

**HPLC:** Shows >99.4% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	62.68	8.16	15.12
Found	62.63	8.07	15.16

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USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373  
www.RnDSYSTEMS.com

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**Description:**

Potent and selective G9a and GLP histone lysine methyltransferase inhibitor ( $IC_{50} < 2.5$  nM). Exhibits >2,000-fold selectivity for G9a and GLP over PRC2-EZH2 and >20,000-fold selectivity over other methyltransferases. Reduces H3K9 dimethylation levels in MDA-MB-231 cells ( $IC_{50} = 110$  nM). Displays modest brain penetration in vivo.

**Physical and Chemical Properties:**

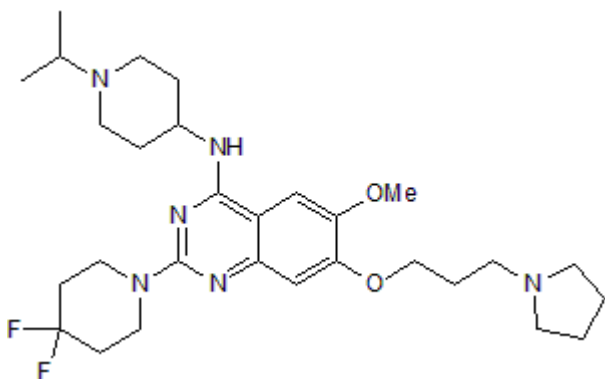
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Batch Molecular Weight: 555.71

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

Liu *et al* (2013) Discovery of an in vivo chemical probe of the lysine methyltransferases G9a and GLP. *J.Med.Chem.* **56** 8931. PMID: 24102134.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

1eq. HCl to 50 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.

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