



# **Certificate of Analysis**

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Product Name: UNC 0638 Catalog No.: 4343 Batch No.: 2

CAS Number: 1255580-76-7

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

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{30}H_{47}N_5O_2.\frac{1}{2}H_2O$ 

Batch Molecular Weight: 509.73

Physical Appearance: Yellow solid

**Solubility:** DMSO to 100 mM

ethanol to 100 mM 3eq. HCl to 100 mM

Storage: Store at +4°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**HPLC:** Shows 98.3% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 69.46 9.33 13.5 Found 69.61 9.26 13.44



## **Product Information**

Print Date: Mar 17th 2020

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## **Description:**

Selective inhibitor of G9a and GLP histone lysine methyltransferases ( $IC_{50}$  values are < 15 nM and 19 nM for G9a and GLP respectively, and > 10000 nM for a range of other histone methyltransferases). Potently inhibits dimethylation of H3K9 in MCF-7 cells ( $IC_{50}$  = 70 nM). Restores metabolic and antiviral function in exhausted CD8+ T cells from patients with chronic HCV infection. Cell permeable.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>30</sub>H<sub>47</sub>N<sub>5</sub>O<sub>2</sub>.½H<sub>2</sub>O

Batch Molecular Weight: 509.73 Physical Appearance: Yellow solid

**Minimum Purity**: ≥98%

#### **Batch Molecular Structure:**

Storage: Store at +4°C

## Solubility & Usage Info:

DMSO to 100 mM ethanol to 100 mM 3eq. HCl 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.

## **Licensing Information:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the UNC 0638 probe summary on the SGC website.

## References:

Barili et al (2020) Targeting p53 and histone methyltransferases restores exhausted CD8+ T cells in HCV infection. Nat.Commun. 11 604. PMID: 32001678.

**Liu** *et al* (2011) Optimization of cellular activity of G9a inhibitors 7-aminoalkoxy-quinazolines. J.Med.Chem. *54* 6139. PMID: 21780790. **Vedadi** *et al* (2011) A chemical probe selectively inhibits G9a and GLP methyltransferase activity in cells. Nat.Chem.Biol. *7* 566. PMID: 21743462.

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