UNC 0631

Cat. No.: HY-13808

CAS No.: 1320288-19-4

Molecular Formula: $C_{37}H_{61}N_7O_2$

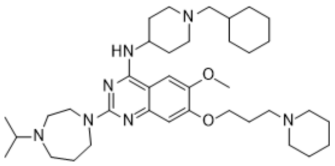
Molecular Weight: 635.93

Target: Histone Methyltransferase

Pathway: Epigenetics

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMF : 150 mg/mL (235.88 mM; Need ultrasonic)
Ethanol : 100 mg/mL (157.25 mM; Need ultrasonic)
DMSO : 16.67 mg/mL (26.21 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.5725 mL	7.8625 mL	15.7250 mL
5 mM	0.3145 mL	1.5725 mL	3.1450 mL
10 mM	0.1573 mL	0.7863 mL	1.5725 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% EtOH >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.5 mg/mL (3.93 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% EtOH >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (3.93 mM); Clear solution
3. Add each solvent one by one: 10% EtOH >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.93 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.67 mg/mL (2.63 mM); Clear solution
5. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.67 mg/mL (2.63 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

UNC 0631 is a potent histone methyltransferase G9a inhibitor with an IC_{50} of 4 nM. UNC 0631 potently reduces H3K9me2

	levels in MDA-MB-231 cells with an IC_{50} of 25 nM[1].
IC_{50} & Target	G9a 4 nM (IC_{50})
In Vitro	UNC 0631 (Compound 7) has high cellular potency and excellent separation of functional potency versus cell toxicity in a variety of cell lines. UNC 0631 is highly potent in reducing H3K9me2 levels and has low cell toxicity. UNC 0631 reduces H3K9me2 levels with ICW IC_{50} values of 25 nM, 18 nM, 26 nM, 24 nM, 51 nM, 72 nM and 46 nM in MDA-MB-231, MCF7, PC3, 22RV1, HCT116 wt, HCT 116 $p53^{-/-}$ and IMR90 cell lines, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- bioRxiv. 2020 Jun.
- Patent. US20180263995A1.

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REFERENCES

[1]. Liu F, et al. Optimization of cellular activity of G9a inhibitors 7-aminoalkoxy-quinazolines. J Med Chem. 2011 Sep 8;54(17):6139-50.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA