Print Date: Mar 23rd 2021

Certificate of Analysis

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Product Name: **UNC 0642** **Catalog No.: 5132** **Batch No.: 2**

CAS Number: 1481677-78-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{44}F_2N_6O_2.½H_2O$

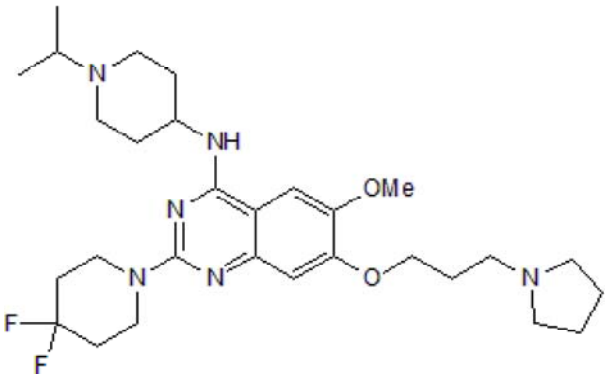
Batch Molecular Weight: 555.71

Physical Appearance: White solid

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

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (9:1:90 MeOH:NH4OH:DCM)

HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.68	8.16	15.12
Found	62.33	8.1	15.01

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Description:

UNC 0642 is a potent and selective G9a and GLP histone lysine methyltransferase inhibitor (IC_{50} < 2.5 nM) that exhibits >2,000-fold selectivity for G9a and GLP over PRC2-EZH2 and >20,000-fold selectivity over other methyltransferases. UNC 0642 reduces H3K9 dimethylation levels in MDA-MB-231 cells (IC_{50} = 110 nM), and displays modest brain penetration in vivo.

Physical and Chemical Properties:

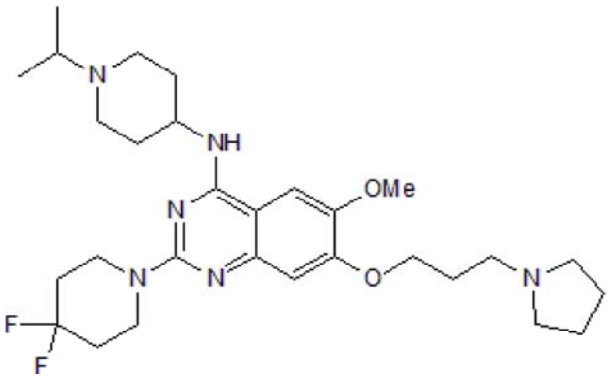
Batch Molecular Formula: $C_{29}H_{44}F_2N_6O_2.½H_2O$

Batch Molecular Weight: 555.71

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at -20°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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the UNC 0642 probe summary on the SGC website.

References:

Scheer *et al* (2019) A chemical biology toolbox to study protein methyltransferases and epigenetic signaling. Nat.Commun. ***10*** 19. PMID: 30604761.

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.