# Data Sheet

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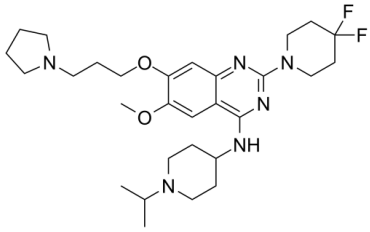
| **Product Name:** | UNC0642 |
| **Cat. No.:** | CS-5269 |
| **CAS No.:** | 1481677-78-4 |
| **Molecular Formula:** | C29H44F2N6O2 |
| **Molecular Weight:** | 546.70 |
| **Target:** | Histone Methyltransferase; Sigma Receptor |
| **Pathway:** | Epigenetics; GPCR/G Protein; Neuronal Signaling |
| **Solubility:** | DMSO : 295 mg/mL (539.60 mM; Need ultrasonic and warming) |



## BIOLOGICAL ACTIVITY:

UNC0642 is a potent and selective **G9a/GLP** inhibitor, inhibits G9a/GLP with an **$IC_{50}$** of less than 2.5 nM. IC50 & Target: IC50: less than 2.5 nM (G9a, GLP)[1] **In Vitro:** UNC0642 displays high in vitro and cellular potency, low cell toxicity, and excellent selectivity. UNC0642 is competitive with the peptide substrate and non-competitive with the cofactor SAM. The $K_i$ of UNC0642 is determined to be 3.7±1 nM. UNC0642 displays high in vitro potency for GLP ($IC_{50}$< 2.5 nM), similar to G9a. UNC0642 is more than 300-fold selective for G9a and GLP over a broad range of kinases, GPCRs, transporters, and ion channels. UNC0642 exhibits high potency at reducing the H3K9me2 mark, low cell toxicity, and good separation of functional potency and cell toxicity in a number of cell lines. It reduces clonogenicity in PANC-1 cells, a pancreatic carcinoma cell line[1]. **In Vivo:** A single intraperitoneal (IP) injection (5 mg/kg) of UNC0642results in a plasma $C_{max}$ (maximum concentration) of 947 ng/mL and an AUC (area under the curve) of 1265 hr*ng/mL[1].

## PROTOCOL (Extracted from published papers and Only for reference)

**Cell Assay:** [1]MDA-MB-231, PC3, and U2OS cells are treated with inhibitors (UNC0642) for 48 h. Cell viability assays are performed by incubating cells with 0.1 mg/mL of resazurin for 3 – 4 h. Resazurin reduction is monitored with 544 nm excitation, measuring fluorescence at 590 nm. In-cell western assay is performed as described previously[1]. **Animal Administration:** [1]Mice: Standard PK studies are performed using male Swiss albino mice. Plasma and brain concentrations are measured at 0.08, 0.25, 0.5, 1, 2, 4, 8, and 24 h following a single IP injection of UNC0642 at 5 mg/kg. The compound concentration at each time point in plasma or brain is the average value from 3 test animals[1].

## References:

[1]. Liu F, et al. Discovery of an in vivo chemical probe of the lysine methyltransferases G9a and GLP. J Med Chem. 2013 Nov 14;56(21):8931-8942.

[2]. Wang L, et al. Targeting EHMT2 reverses EGFR-TKI resistance in NSCLC by epigenetically regulating the PTEN/AKT signaling pathway. Cell Death Dis. 2018 Jan 26;9(2):129

## CAIndexNames:

4-Quinazolinamine, 2-(4,4-difluoro-1-piperidinyl)-6-methoxy-N-[1-(1-methylethyl)-4-piperidinyl]-7-[3-(1-pyrrolidinyl)propoxy]-

## SMILES:

CC(N1CCC(NC2=C3C=C(OC)C(OCCCN4CCCC4)=CC3=NC(N5CCC(F)(F)CC5)=N2)CC1)C

**Caution: Product has not been fully validated for medical applications. For research use only.**

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