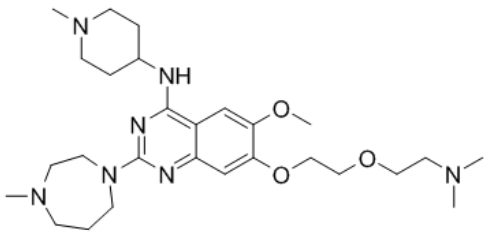
Product Data Sheet

Product Name: UNC0321
Cat. No.: GC37856

Chemical Properties

Cas. No.	1238673-32-9		
SMILES	CN1CCC(NC2=C3C=C(OC)C(OCCOCCN(C)C)=CC3=NC(N4CCN(C)CCC4)=N2)CC1		
Formula	$C_{27}H_{45}N_7O_3$	M.Wt	515.69
Solubility	DMSO: ≥ 31 mg/mL (60.11 mM)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure			



Background

UNC0321 is a potent and selective G9a inhibitor with Ki of 63 pM, UNC0321 is the first G9a inhibitor with picomolar potency and the most potent G9a inhibitor to date.IC50 value: 63 pM(Ki); 9 nM (ECSD assay) [1]Target: G9aIt was found that replacing the 5-carbon chain in compound 13 with an ethoxyethyl chain resulted in compound 29{UNC0321} (IC50 = 6 nM (CLOT) and 9 nM (ECSD)), the most potent G9a inhibitor to date. 29 had a Morrison Ki of 63 pM and was about 40-fold more potent than 10 (Morrison Ki = 2.6 nM) and 250-fold more potent than 3a (Morrison Ki = 16 nM) in this G9a assay. UNC0321 potentially useful small molecule tools for the biomedical research community to

investigate the biology of G9a and its role in chromatin remodeling as well as PTMs of other proteins.

[1]. Liu F, et al. Protein lysine methyltransferase G9a inhibitors: design, synthesis, and structure activity relationships of 2,4-diamino-7-aminoalkoxy-quinazolines. J Med Chem. 2010 Aug 12;53(15):5844-57. [2]. Liu F, et al. Optimization of cellular activity of G9a inhibitors 7-aminoalkoxy-quinazolines. J Med Chem. 2011 Sep 8;54(17):6139-50.