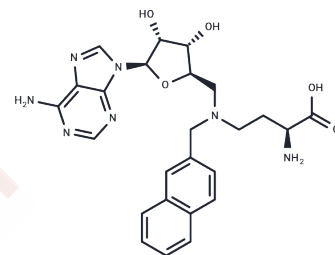


Bisubstrate Inhibitor 78

Chemical Properties

CAS No. :	2368247-39-4
Formula:	C ₂₅ H ₂₉ N ₇ O ₅
Molecular Weight:	507.54
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year Actual storage temperature shall be subject to the COA.



Biological Description

Description	Bisubstrate inhibitor 78 is an inhibitor of nicotinamide N-methyltransferase (NNMT; IC ₅₀ = 1.41 μM). It binds the NNMT active site in the binding pockets for the NNMT substrates S-adenosyl-L-methionine (SAM) and nicotinamide. Bisubstrate inhibitor 78 is selective for NNMT over histone-lysine N-methyltransferase NSD2 and protein arginine methyltransferase 1 (PRMT1; IC ₅₀ s = >50 μM for both). It reduces levels of 1-methylnicotinamide in, and inhibits proliferation of, HSC-2 oral cancer cells when used at a concentration of 100 μM. This compound is unstable in powder form and other related salt forms are recommended.
Targets(IC ₅₀)	Others

Solubility Information

Solubility	DMF: Slightly soluble Chloroform: Slightly soluble Ethanol: Slightly soluble DMSO: Slightly soluble Methanol: Slightly soluble (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9703 mL	9.8514 mL	19.7029 mL
5 mM	0.3941 mL	1.9703 mL	3.9406 mL
10 mM	0.197 mL	0.9851 mL	1.9703 mL
50 mM	0.0394 mL	0.197 mL	0.3941 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Gao, Y., van Haren, M.J., Moret, E.E., et al. Bisubstrate inhibitors of nicotinamide N-methyltransferase (NNMT) with enhanced activity. *J. Med. Chem.* 62(14)6597-6614(2019)

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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