

Product Data Sheet

Product Name: Bisubstrate Inhibitor 78

Cat. No.: GC48463

Chemical Properties

Cas. No. 2368247-39-4

SMILES OC([C@@H](N)CCN(CC1=CC(C=CC=C2)=C2C=C1)C[C@@H]3[C@@H](O)[C@@H](O)[C@H](N4C5=NC=NC(N)=C5N=C4)O3)=O

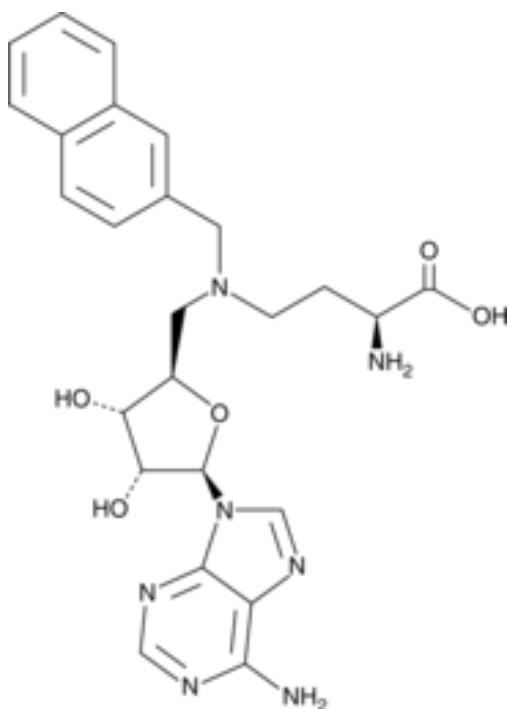
Formula C₂₅H₂₉N₇O₅ M.Wt 507.5

Solubility Chloroform: slightly soluble, DMF: slightly soluble, DMSO: slightly soluble, Ethanol: slightly soluble, Methanol: slightly soluble
Storage -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



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

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Background

Bisubstrate inhibitor 78 is an inhibitor of nicotinamide N-methyltransferase (NNMT; $IC_{50} = 1.41 \mu M$).¹ 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; $IC_{50}s = >50 \mu M$ for both). It reduces levels of 1-methylnicotinamide in, and inhibits proliferation of, HSC-2 oral cancer cells when used at a concentration of $100 \mu M$.

1. 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)

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