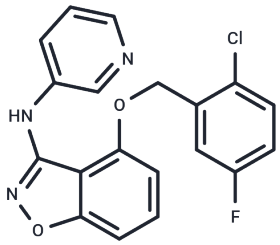
Data Sheet (Cat.No.T7263)

TargetMol

SMS2-IN-2

Chemical Properties



CAS No. : 2241838-28-6

Formula: C19H13ClFN3O2

Molecular Weight: 369.78

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	SMS2-IN-2 (SMS2 inhibitors) is a potent, selective and orally active sphingomyelin synthase 2 (SMS2) inhibitor, (IC50s of 100 and 56 μM for SMS2 and SMS1, respectively). SMS2-IN-2 has anti-chronic inflammatory activity.
Targets(IC50)	Others,Phospholipase

Solubility Information

Solubility	DMSO: 250 mg/mL (676.08 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (13.52 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.7043 mL	13.5216 mL	27.0431 mL
5 mM	0.5409 mL	2.7043 mL	5.4086 mL
10 mM	0.2704 mL	1.3522 mL	2.7043 mL
50 mM	0.0541 mL	0.2704 mL	0.5409 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

Mo M, Yang J, Jiang XC,et al.Discovery of 4-Benzyloxybenzo[d]isoxazole-3-amine Derivatives as Highly Selective and Orally Efficacious Human Sphingomyelin Synthase 2 Inhibitors that Reduce Chronic Inflammation in db/ db Mice[J].J Med Chem. 2018 Sep 27;61(18):8241-8254.

Liang H, Ma X, Zhang Y, et al.The formation of migrasomes is initiated by the assembly of sphingomyelin synthase 2 foci at the leading edge of migrating cells.Nature Cell Biology.2023: 1-12.