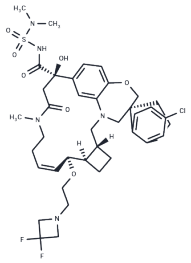
Data Sheet (Cat.No.T11972)

TargetMol

Mcl-1 inhibitor 3

Chemical Properties



CAS No. : 2376774-73-9

Formula: C40H52ClF2N5O7S

Molecular Weight: 820.39

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	Mcl-1 inhibitor 3 shows good pharmacokinetic properties and excellent in vivo efficacy without toxicity.Mcl-1 inhibitor 3 is a highly potent and orally activate macrocyclic Mcl-1 inhibitor (Ki= 0.061 nM; IC50=19 nM in an OPM-2 cell viability assay).
Targets(IC50)	Bcl-2 Family
In vitro	Mcl-1 inhibitor 3 exhibits an IC50 of 19 nM in an OPM-2 cell viability assay and a Ki of 0.061 nM in an Mcl-1 HTRF/TR-FRET assay.
In vivo	Mcl-1 inhibitor 3 (oral administration; 10, 30, or 60 mg/kg; 30 days) led to robust dose-dependent tumor growth inhibition at 30 mg/kg (44% TGI) and 34% tumor regression at 60 mg/kg without any body weight loss in the mice. Mcl-1 inhibitor 3 (oral administration; 3, 10, or 30 mg/kg; 6 hours) resulted in significant luminescence loss (~40%) at 30 mg/kg, with corresponding unbound drug levels in plasma showing [plasma]u/OPM-2 IC50 values of 0.24, 0.93, and 3.65 μM at 3, 10, and 30 mg/kg, respectively. Additionally, Mcl-1 inhibitor 3 (oral administration; 10, 30, or 60 mg/kg; 6 hours) activated Bak by 8-fold at 30 mg/kg and by 14-fold at 60 mg/kg in the OPM-2 Luc assay, based on the detection of activated Bak in nude mice via electrochemiluminescence.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.2189 mL	6.0947 mL	12.1893 mL
5 mM	0.2438 mL	1.2189 mL	2.4379 mL
10 mM	0.1219 mL	0.6095 mL	1.2189 mL
50 mM	0.0244 mL	0.1219 mL	0.2438 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

Rescourio G, Discovery and in Vivo Evaluation of Macrocyclic Mcl-1 Inhibitors Featuring an α-Hydroxy Phenylacetic Acid Pharmacophore or Bioisostere.J Med Chem. 2019 Nov 27;62(22):10258-10271.