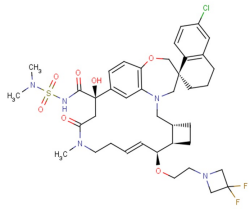
Data Sheet (Cat.No.T11972)

TargetMol
A DRUG SCREENING EXPERT

Mcl-1 inhibitor 3

Chemical Properties



CAS No.:	2376774-73-9
Formula:	C40H52ClF2N5O7S
Molecular Weight:	820.38
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

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(IC_{50})	Mcl-1: 0.061 nM (ki)
In vitro	Mcl-1 inhibitor 3 shows an IC50 value of 19 nM in an OPM-2 cell viability assay, and a Ki value of 0.061 nM in Mcl-1 HTRF/TR-FRET assay.
In vivo	Mcl-1 inhibitor 3 (oral administration; 10, 30, or 60 mg/kg; 30 days) led to a robust dose-dependent tumor growth inhibition at 30 mg/kg (44% TGI) and 34% tumor regression when the animals were dosed at 60 mg/kg.Lastly, no body weight loss is observed in any of the mice in this study efficacy models.Mcl-1 inhibitor 3 (oral administration; 3, 10, or 30 mg/kg; 6 hours) causes a significant loss of luminescence (~40%) over vehicle at 30 mg/kg,This effect was observed with unbound drug levels in plasma, the [plasma]u/OPM-2 IC50 values are 0.24, 0.93 and 3.65 μM in 3, 10, 30 mg/kg doses,respectively. Mcl-1 inhibitor 3 (oral administration; 10, 30, or 60 mg/kg; 6 hours) activates Bak by 8-fold at 30 mg/kg and by 14-fold at 60 mg/kg in this OPM-2 Luc assay,this test is based on the detection of activated Bak in nude mice subcutaneously injected with via electrochemiluminescence.

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.219 mL	6.095 mL	12.189 mL
5 mM	0.244 mL	1.219 mL	2.438 mL
10 mM	0.122 mL	0.609 mL	1.219 mL
50 mM	0.024 mL	0.122 mL	0.244 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. 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.

Tel:781-999-4286 E-mail:info@targetmol.com Address:36 Washington Street,Wellesley Hills,MA 02481