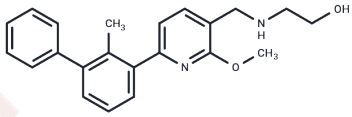
Data Sheet (Cat.No.T9651)

TargetMol

PD-1/PD-L1-IN-9

Chemical Properties



CAS No. : 2628506-54-5

Formula: C22H24N2O2

Molecular Weight: 348.44

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	PD-1/PD-L1-IN-9, with an IC50 of 3.8 nM, is a potent and orally active inhibitor of the PD-1/PD-L1 interaction. It enhances the immune cells' ability to kill tumor cells and demonstrates significant antitumor activity in vivo in a CT26 mouse model.
Targets(IC50)	PD-1/PD-L1
In vitro	PD-1/PD-L1-IN-9 (46.9-1500 nM; pretreated for 2 h) enhances the antitumor immunity of PBMCs against MDB-MB 231 cells in a dose-dependent manner, with an EC50 of approximately 100 nM[1].
In vivo	PD-1/PD-L1-IN-9 (40-80 mg/kg; p.o. once a day for 2 weeks) inhibits tumor growth in a dose-dependent manner without causing body weight loss or mortality in mice. PD-1/PD-L1-IN-9 (3 mg/kg; a single i.v.) exhibits a half-life (t1/2=4.2 h), plasma clearance (Cl=11.5 L/h/kg), and Cmax (1233 ng/mL) in rats. PD-1/PD-L1-IN-9 (25 mg/kg; a single p.o.) shows moderate oral bioavailability (F=22%), half-life (t1/2=6.4 h), and Cmax (192 ng/mL) in rats[1].

Solubility Information

Solubility	DMSO: 90 mg/mL (258.29 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: 3.3 mg/mL (9.47 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	2.8699 mL	14.3497 mL	28.6993 mL
5 mM	0.574 mL	2.8699 mL	5.7399 mL
10 mM	0.287 mL	1.435 mL	2.8699 mL
50 mM	0.0574 mL	0.287 mL	0.574 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

Wang T, et, al. Novel Biphenyl Pyridines as Potent Small-Molecule Inhibitors Targeting the Programmed Cell Death-1/Programmed Cell Death-Ligand 1 Interaction. J Med Chem. 2021 May 30.