Screening Libraries

Product Data Sheet

PD-1/PD-L1-IN-10

Cat. No.: HY-132202 CAS No.: 2487550-41-2 Molecular Formula: $C_{33}H_{31}N_3O_7$

Molecular Weight: 581.62

Target: PD-1/PD-L1; Apoptosis

Pathway: Immunology/Inflammation; Apoptosis

Storage: Powder -20°C

3 years 4°C 2 years

In solvent -80°C 6 months

> -20°C 1 month

SOLVENT & SOLUBILITY

In Vitro

DMSO: 100 mg/mL (171.93 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	1.7193 mL	8.5967 mL	17.1934 mL
	5 mM	0.3439 mL	1.7193 mL	3.4387 mL
	10 mM	0.1719 mL	0.8597 mL	1.7193 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (4.30 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	PD-1/PD-L1-IN-10 (compound B2) is an orally active PD-1/PD-L1 inhibitor (IC ₅₀ of 2.7 nM) with potent anticancer efficacy ^[1] .
IC ₅₀ & Target	IC50: 2.7 nM (PD-1/PD-L1) ^[1] .
In Vitro	PD-1/PD-L1-IN-10 (compound B2) significantly promotes interferongamma secretion in a dose-dependent manner in vitro even at the low concentration of 1 nM ^[1] . PD-1/PD-L1-IN-10 (compound B2) does not affect cell viability of LLC cells and lymph node T-cells ^[1] . PD-1/PD-L1-IN-10 (compound B2, 0-100 nM) stabilizes the PD-L1 protein in mouse Lewis lung carcinoma (LLC) cells. In particular, PD-1/PD-L1-IN-10 (compound B2) maintains the PD-L1 stability in a dose-dependent manner at 58 °C. Suggesting that PD-1/PD-L1-IN-10 (compound B2) could enter LLC cells and then directly binds to the PD-L1 protein ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

PD-1/PD-L1-IN-10 (compound B2, 5 mg/kg, intragastric gavage) exhibits potent in vivo anticancer efficacy in an LLC-bearing allograft mouse model. PD-1/PD-L1-IN-10 (compound B2) effectively blocks tumor cell proliferation and induces apoptosis in LLC tumor tissues. [1].

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Animal Model:	LLC tumor-bearing mice $^{[1]}$.	
Dosage:	2, 5 mg/kg.	
Administration:	i.g., qd., for 21 days	
Result:	Significantly suppressed the growth of the tumor in a dose-dependent manner compared with the vehicle group.	

REFERENCES

[1]. Yiqiang OuYang, et al. Design, Synthesis, and Evaluation of o-(Biphenyl-3-ylmethoxy)nitrophenyl Derivatives as PD-1/PD-L1 Inhibitors with Potent Anticancer Efficacy In Vivo. J Med Chem. 2021 May 26.

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

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