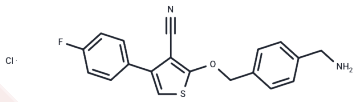
Data Sheet (Cat.No.T79314)

TargetMol

PD-L1-IN-3

Chemical Properties



CAS No. :	2953044-29-4
Formula:	C19H15ClFN2OS
Molecular Weight:	373.85
Storage:	Store at low temperature 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-L1-IN-3 (Compound 4a) functions as an inhibitor of the PD-1/PD-L1 axis, with an IC50 value of 4.97 nM for PD-L1 inhibition and an EC50 value of 2.70 μM for Jurkat T cell modulation. It antagonizes the PD-1/PD-L1 interaction by binding to the PD-L1 dimer, obstructing PD-1 signaling. This compound is utilized in research pertaining to lung cancer and melanoma [1].
Targets(IC50)	PD-1/PD-L1
In vitro	PD-L1-IN-3 (Compound 4a) disrupts the PD-1 and PD-L1 interaction at concentrations of 0.01 to 100 μM over 40 minutes, enhancing TCR-mediated activation of Jurkat cells [1]. Additionally, PD-L1-IN-3 demonstrates increased uptake in PD-L1-positive H358 tumors, proportional to PD-L1 expression levels [1].
In vivo	In PD-L1+/– (H358 and ES2) tumors, PD-L1-IN-3 (0.01-100 μM; incubation) was observed to exhibit 40-55% higher uptake in PD-L1+ H358 tumors compared to wild-type counterparts. However, it failed to distinguish between wild-type and knockout ES2 samples[1].

Solubility Information

Solubility	DMSO: 100 mg/mL (267.49 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6749 mL	13.3743 mL	26.7487 mL
5 mM	0.535 mL	2.6749 mL	5.3497 mL
10 mM	0.2675 mL	1.3374 mL	2.6749 mL
50 mM	0.0535 mL	0.2675 mL	0.535 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

Ważyńska MA, et al. Design, Synthesis, and Biological Evaluation of 2-Hydroxy-4-phenylthiophene-3-carbonitrile as PD-L1 Antagonist and Its Comparison to Available Small Molecular PD-L1 Inhibitors. J Med Chem. 2023 Jul 27;66 (14):9577-9591.