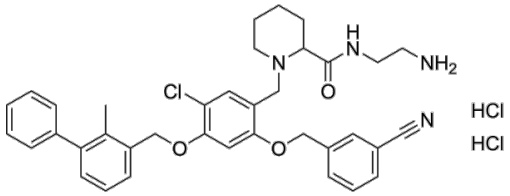
Product Data Sheet

Product Name: PD-1/PD-L1-IN-63
Cat. No.: GC79374

Chemical Properties

Cas. No.	2691796-92-4		
Formula	$C_{37}H_{41}Cl_3N_4O_3$	M.Wt	696.11
Solubility	DMSO: 104 mg/mL (149.40 mM; Need ultrasonic)	Storage	Store at 4°C, stored under nitrogen, away from moisture
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure			



Background

PD-1/PD-L1-IN-63 is an orally active PD-1/PD-L1 inhibitor with an IC_{50} of 9.1 nM. PD-1/PD-L1-IN-63 blocks the PD-1/PD-L1 interaction, induces cancer cell death and inhibits tumor growth. PD-1/PD-L1-IN-63 can be used in the research of melanoma [1].

In Vivo, PD-1/PD-L1-IN-63 (50-100 mg/kg; i.g.; 14 days) exhibits potent dose-dependent antitumor activity in humanized PD-1 C57BL/6J mice inoculated with B16-F10 melanoma[1]. PD-1/PD-L1-IN-63 (50-100 mg/kg; i.g.; 14 days) does not induce cardiotoxicity or myelosuppression in healthy BALB/c

mice when administered via oral gavage at doses of 50 or 100 mg/kg once daily for 14 days[1].

In Vitro, PD-1/PD-L1-IN-63 potently inhibits PD-1/PD-L1 protein interaction with an IC_{50} of 9.1 nM in an HTRF binding assay[1]. PD-1/PD-L1-IN-63 binds to both purified human PD-L1 (KD = 88.3 nM) and murine PD-L1 (KD = 174 nM) proteins with similar high affinities as measured by ITC[1]. PD-1/PD-L1-IN-63 (0.05-5 μM) binds dose-dependently to purified human PD-L1 (KD = 202 nM) and murine PD-L1 (KD = 471 nM) proteins as measured by SPR[1]. PD-1/PD-L1-IN-63 (37-1000 nM; 48 h) promotes HepG2 cell death in a dose-dependent manner in a HepG2/hPD-L1 and Jurkat/hPD-1 coculture cell model, increasing HepG2 mortality by 58.2% at 1000 nM[1]. PD-1/PD-L1-IN-63 (48 h) inhibits the proliferation of MCF-7, H1299, HeLa, HepG2, and Jurkat cells in vitro with IC_{50} values ranging from 2.3 μM to 4.1 μM[1].

References:
[1]. Cheng B, et al. Discovery of Novel and Highly Potent Resorcinol Dibenzyl Ether-Based PD-1/PD-L1 Inhibitors with Improved Drug-like and Pharmacokinetic Properties for Cancer Treatment. J Med Chem. 2020 Dec 24;63(24):15946-15959.