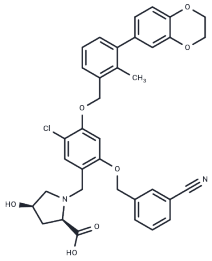
Data Sheet (Cat.No.T5697)

TargetMol

BMS-1166

Chemical Properties



CAS No. : 1818314-88-3

Formula: C36H33ClN2O7

Molecular Weight: 641.11

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	BMS-1166 is a potent inhibitor of the PD-1/PD-L1 interaction.
Targets(IC50)	PD-1/PD-L1
In vitro	BMS-1166 alleviate the inhibitory effect of the soluble PD-L1 on the T-cell receptor-mediated activation of T-lymphocytes. Moreover, the compounds were effective in attenuating the inhibitory effect of the cell surface-associated PD-L1.
Kinase Assay	Purified proteins in 10 mM Tris (pH 8.0) containing 20 mM NaCl, were concentrated to 5 mg/ml, mixed with the inhibitor in 1:3 molar ratio (protein:compound) and clarified by centrifugation at 15 000 × g for 10 min. Supernatant was used for screening using a sitting-drop vapor diffusion method. Diffraction-quality crystals were obtained at room temperature from 0.1 M Tris pH 8.5 containing 0.2 M magnesium chloride and 30% (w/v) PEG 4000 for the hPD-L1/BMS-1001 complex and from 0.01 M Tris pH 8.4 containing 0.28 M sodium chloride and 27% (w/v) PEG 4000 for hPD-L1/BMS-1166 complex.

Solubility Information

Solubility	DMSO: 245 mg/mL (382.15 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: < 10 mg/mL (15.6 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+90% Corn oil: < 10 mg/mL (15.6 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+90% Saline: < 10 mg/mL (15.6 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+90% (20% SBE-β-CD in Saline): < 10 mg/mL (15.6 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. *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	1.5598 mL	7.799 mL	15.5979 mL
5 mM	0.312 mL	1.5598 mL	3.1196 mL
10 mM	0.156 mL	0.7799 mL	1.5598 mL
50 mM	0.0312 mL	0.156 mL	0.312 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

Skalniak L , Zak K M , Guzik K , et al. Small-molecule inhibitors of PD-1/PD-L1 immune checkpoint alleviate the PD-L1-induced exhaustion of T-cells[J]. Oncotarget, 2017, 8(42).