BMS-8

Cat. No.: HY-116274

CAS No.: 1675201-90-7

Molecular Formula: $C_{27}H_{28}BrNO_3$

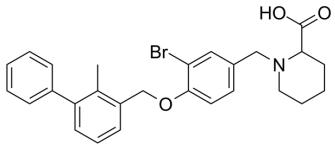
Molecular Weight: 494.42

Target: PD-1/PD-L1

Pathway: Immunology/Inflammation

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 83.33 mg/mL (168.54 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0226 mL	10.1129 mL	20.2257 mL
	5 mM	0.4045 mL	2.0226 mL	4.0451 mL
	10 mM	0.2023 mL	1.0113 mL	2.0226 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: ≥ 2.08 mg/mL (4.21 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.21 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BMS-8 inhibits the PD-1/PD-L1 interaction with IC_{50} of 7.2 μM. BMS-8, binds directly to PD-L1 and induces formation of PD-L1 homodimers, which in turn prevents the interaction with PD-1[1].

In Vitro

BMS-8 tends to have a more stable binding mode with one PD-L1 monomer than the other and the small-molecule inducing PD-L1 dimerization was further stabilized by the non-polar interaction of Ile54, Tyr56, Met115, Ala121, and Tyr123 on both monomers and the water bridges involved in ALys124[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Eun-Hye Kim, et al. Preparation of Biphenyl-Conjugated Bromotyrosine for Inhibition of PD-1/PD-L1 Immune Checkpoint Interactions. Int J Mol Sci. 2020 May 21;21(10):3639.

[2]. Danfeng Shi, et al. Computational Insight Into the Small Molecule Intervening PD-L1 Dimerization and the Potential Structure-Activity Relationship. Front Chem. 2019 Nov 12;7:764.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA