BMS-8

Cat. No.: HY-116274

CAS No.: 1675201-90-7

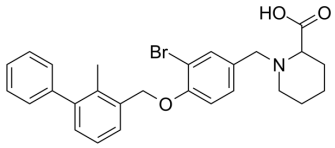
Molecular Formula: $C_{27}H_{28}BrNO_3$

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	Solvent / Mass / 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.

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.

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

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