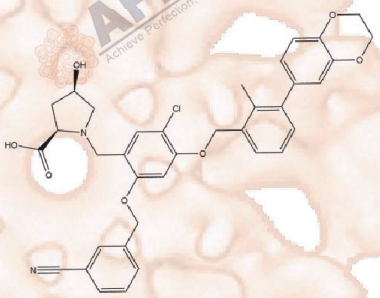
Product Data Sheet

BMS-1166



Cat. No.: BA6141

CAS No.: 1818314-88-3

Formula: C36H33ClN2O7

M.Wt: 641.11

Synonyms: (4R)-1-[[5-chloro-2-[(3-cyanophenyl)methoxy]-4-[[3-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-methylphenyl]methoxy]phenyl]methyl]-4-hydroxy-D-proline

Target: PD-1/PD-L1

Pathway: Cell Cycle/DNA Damage

Storage: Store at -20° C

Solvent & Solubility

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In Vitro — Preparing Stock Solutions

Concentration \ Solvent \ Mass	1mg	5mg	10mg
1 mM	1.5598 mL	7.7990 mL	15.5979 mL
5 mM	0.3120 mL	1.5598 mL	3.1196 mL
10 mM	0.1560 mL	0.7799 mL	1.5598 mL

Please refer to the solubility information to select the appropriate solvent.

Biological Activity

Shortsummary

BMS-1166 (CAS 1818314-88-3) is a small-molecule immune checkpoint inhibitor, functioning as a potent antagonist in T cell activation and exhibiting strong inhibitory activity against the interaction between PD-1 and its ligand PD-L1 in immune cells. Additionally, it disrupts immune checkpoint signaling pathways by inducing dimerization and thereby blocks the engagement of programmed cell death protein 1 (PD-1) with its ligand.

	In in vitro experimental assays, BMS-1166 demonstrates efficient inhibition of the PD-1/PD-L1 binding with an IC50 value of 1.4 nM, tested against cellular models expressing human checkpoint proteins. It can also reverse the immune suppression mediated by the PD-1/PD-L1 axis, leading to enhanced T cell proliferation and cytokine release. In immuno-oncology research and drug development, BMS-1166 is widely used for studying the therapeutic potential of immune checkpoint blockade, specifically focusing on antitumor immunity. Its application facilitates the evaluation of immune checkpoint-targeted strategies and accelerates preclinical investigations aimed at restoring or augmenting immune responses against cancer.
IC_{50} & Target	

In Vitro

Cell Viability Assay

Cell Line:	CHO
Preparation method:	Growth inhibition of CHO cells expressing PDL-1/TCRa measured after 24 h co-culturing with human Jurkat cells expressing PD-1/NFAT-Luc in presence of compound by Cell Titer-Glo luminescent cell viability assay
Reacting conditions:	1 nM-0.1 mM, 37° C, 24 h
Applications:	GI50> 30 μM

In Vivo

Animal experiment

Animal models:	SCID mice, BalB/c mice
Dosage form:	Oral formulation concentration: Prepared to a final concentration of 0.5 mg/ml. For SCID mice (with human HCC MHCC97-H cells and human PBL infusion), BMS-1166 was tested at 0.2, 0.5, 1, 2, 5, 10 mg/kg. For BalB/c mice (with mouse HCC H22 cells), doses were 0.5, 1, 2, 5, 10, 20 mg/kg.
Applications:	BMS-1166 inhibited HCC growth. BMS-1166 + SNM significantly reduced tumor volume and weight vs. BMS-1166 alone ($p<0.05$).
Preparation method:	20 – 50 mg of BMS-1166 pure powder was weighed and mixed with polyethylene glycol 400, Tween 80, and a small volume of dimethyl sulfoxide (assisted by ultrasound and vortex mixing). After dissolution, sterilized 0.9% saline was added, stirred and shaken to prepare an oral formulation, which was filtered through a 0.22 μm pre-sterilized membrane, aliquoted into pre-sterilized 10-ml centrifuge tubes, stored at −80 ° C, and kept at 4 ° C away from light during experiments.
Other notes:	The technical data provided above is for reference only.

Product Citations

References

1. Chen H, Wang K, Yang Y, Huang X, Dai X, Feng Z. Design, synthesis, and structure-activity relationship of programmed cell death-1/programmed cell death-ligand 1 interaction inhibitors bearing a benzo[d]isothiazole scaffold. Eur J Med Chem. 2021 May 5;217:113377. doi: 10.1016/j.ejmech.2021.113377. Epub 2021 Mar 15. PMID: 33770574.

2. Mao D, Xu M, Jiang Q, Sun H, Sun F, Yang R, Chai Y, Li X, Li B, Li Y. A Single Nucleotide Mixture Enhances the Antitumor Activity of Molecular-Targeted Drugs Against Hepatocellular Carcinoma. Front Pharmacol. 2022 Jun 27;13:951831. doi: 10.3389/fphar.2022.951831. PMID: 35833031; PMCID: PMC9271877.

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most APExBIO products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

APExBIO Technology

www.apexbt.com

7505 Fannin street, Suite 410, Houston, TX 77054.

Tel: +1-832-696-8203 | Fax: +1-832-641-3177 | Email: info@apexbt.com