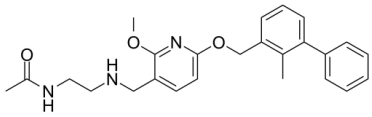
Data Sheet

Product Name:	BMS-202
Cat. No.:	CS-5441
CAS No.:	1675203-84-5
Molecular Formula:	C25H29N3O3
Molecular Weight:	419.52
Target:	Apoptosis; PD-1/PD-L1
Pathway:	Apoptosis; Immunology/Inflammation
Solubility:	DMSO : ≥ 100 mg/mL (238.37 mM)



BIOLOGICAL ACTIVITY:

BMS-202 is a potent and nonpeptidic **PD-1/PD-L1 complex** inhibitor with an **IC_{50}** of 18 nM and a **K_D** of 8 μM. BMS-202 binds to PD-L1 and blocks human PD-1/PD-L1 interaction. BMS-202 has antitumor activity[1][2]. IC50 & Target: IC50: 18 nM (PD-1/PD-L1)[1] KD: 8 μM (PD-1/PD-L1)[1] **In Vitro:** BMS-202 (0-100 μM; 4 days; SCC-3 or Jurkat cells) treatment inhibits the proliferation of strongly PD-L1-positive SCC-3 cells (IC_{50} of 15 μM) and anti-CD3 antibody-activated Jurkat cells (IC_{50} 10 μM) in vitro[2].
BMS-202 selectively induces thermal stabilization of PD-L1. BMS-202 induces dimerization of PD-L1 in solution.BMS-202 is located at the center of the homodimer filling a deep hydrophobic pocket contributing multiple additional interactions between the monomers. BMS-202 interacts with both PD-L1 molecules using hydrophobic surfaces physiologically involved in the PD-1/PD-L1 interaction[1]. **In Vivo:** BMS-202 (20 mg/kg; intraperitoneal injection; daily; for 9 days; NOG-dKO mice) treatment shows a clear antitumor effect compared with the controls, in humanized MHC- dKO NOG mice[2].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]All binding studies are performed in an HTRF assay buffer consisting of dPBS supplemented with 0.1% (with v) bovine serum albumin and 0.05% (v/v) Tween-20. For the PD-l-Ig/PD-Ll-His binding assay, inhibitors are pre-incubated with PD-Ll-His (10 nM final) for 15 m in 4 μL of assay buffer, followed by addition of PD-l-Ig (20 nM final) in 1 μL of assay buffer and further incubation for 15 m. PD-L1 from either human, cyno, or mouse are used. HTRF detection is achieved using europium crypate-labeled anti- Ig (1 nM final) and allophycocyanin (APC) labeled anti-His (20 nM final). Antibodies are diluted in HTRF detection buffer and 5 μL is dispensed on top of binding reaction. The reaction mixture is allowed to equilibrate for 30 minutes and signal (665 nm/620 nm ratio) is obtained using an En Vision fluorometer. Additional binding assays are established between PD-1-Ig/PD-L2-His (20, 5 nM, respectively), CD80-His/PD-Ll-Ig (100, 10 nM, respectively) and CD80-His/CTLA4-Ig (10, 5 nM, respectively).

References:

[1]. Zak KM, et al. Structural basis for small molecule targeting of the programmed death ligand 1 (PD-L1). Oncotarget. 2016 May 24;7(21):30323-35.

[2]. Ashizawa T, et al. Antitumor activity of the PD-1/PD-L1 binding inhibitor BMS-202 in the humanized MHC-double knockout NOG mouse. Biomed Res. 2019;40(6):243-250.

CAIndexNames:

Acetamide, N-[2-[[[2-methoxy-6-[(2-methyl[1,1'-biphenyl]-3-yl)methoxy]-3-pyridinyl]methyl]amino]ethyl]-

SMILES:

CC(NCCNCC1=CC=C(OCC2=C(C)C(C3=CC=CC=C3)=CC=C2)N=C1OC)=O

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

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