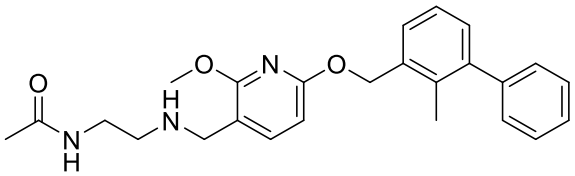
Product data sheet

MedKoo Cat#: 561499 Name: BMS-202 CAS#: 1675203-84-5 Chemical Formula: $C_{25}H_{29}N_3O_3$ Exact Mass: 419.2209 Molecular Weight: 419.52	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
BMS-202 is a PD-1/PD-L1 interaction inhibitor. BMS-202 binds to and induces dimerization of PD-L1, an inhibitory immune checkpoint protein.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	62.0	146.99

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.83 mL	11.92 mL	23.84 mL
5 mM	0.48 mL	2.38 mL	4.77 mL
10 mM	0.24 mL	1.19 mL	2.38 mL
50 mM	0.05 mL	0.24 mL	0.48 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Ashizawa T, Iizuka A, Tanaka E, Kondou R, Miyata H, Maeda C, Sugino T, Yamaguchi K, Ando T, Ishikawa Y, Ito M, Akiyama Y. 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. doi: 10.2220/biomedres.40.243. PMID: 31839668.
2. Hu Z, Yu P, Du G, Wang W, Zhu H, Li N, Zhao H, Dong Z, Ye L, Tian J. PCC0208025 (BMS202), a small molecule inhibitor of PD-L1, produces an antitumor effect in B16-F10 melanoma-bearing mice. PLoS One. 2020 Mar 26;15(3):e0228339. doi: 10.1371/journal.pone.0228339. Erratum in: PLoS One. 2021 Apr 28;16(4):e0251020. PMID: 32214351; PMCID: PMC7098565.

In vivo study

1. Ashizawa T, Iizuka A, Tanaka E, Kondou R, Miyata H, Maeda C, Sugino T, Yamaguchi K, Ando T, Ishikawa Y, Ito M, Akiyama Y. 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. doi: 10.2220/biomedres.40.243. PMID: 31839668.
2. Hu Z, Yu P, Du G, Wang W, Zhu H, Li N, Zhao H, Dong Z, Ye L, Tian J. PCC0208025 (BMS202), a small molecule inhibitor of PD-L1, produces an antitumor effect in B16-F10 melanoma-bearing mice. PLoS One. 2020 Mar 26;15(3):e0228339. doi: 10.1371/journal.pone.0228339. Erratum in: PLoS One. 2021 Apr 28;16(4):e0251020. PMID: 32214351; PMCID: PMC7098565.

Product data sheet

7. Bioactivity

Biological target:

BMS-202 is a potent and nonpeptidic PD-1/PD-L1 complex inhibitor with an IC50 of 18 nM and a KD of 8 μM.

In vitro activity

In order to investigate cytotoxicity of PCC0208025 (BMS202), both tumor cells and CD3+ cells were exposed to different concentrations of PCC0208025. The results in Table 1 showed that IC50 were above 10.0 μM to mice tumor cells and human CD3+ cells, which indicates PCC0208025 possesses low cytotoxicity in vitro. The effects of PCC0208025 on the production of cytokine IFN-γ in human CD3+ cells in vitro were also investigated. As shown in Fig 3, combined aCD3 and aCD28 significantly increased the IFN-γ expression compared with medium control (each treatment $P < 0.05$, $n = 6$), which was significantly decreased by human PD-L1 protein (each treatment $P < 0.05$, $n = 6$). However, anti-PD-L1 antibody BMS-936559 and the compound PCC0208025 from 0.01 to 1 μM markedly rescued PD-L1-mediated inhibition of IFN-γ production (each treatment $P < 0.05$, respectively, $n = 6$).

PLoS One. 2020; 15(3): e0228339. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7098565/

In vivo activity

The anti-cancer activities of PCC0208025 in B16-F10-bearing mice was investigated. It was found that treatment with PCC0208025 at 30 mg/kg and 60 mg/kg significantly decreased tumor weight ($P < 0.05$, $n = 8$) and tumor volumes (day 20, $P < 0.05$, $n = 8$) compared with the control group (Fig 4A and 4B). According to tumor weight, 30 mg/kg and 60 mg/kg of PCC0208025 presented the IR of 30.3% and 50.1%, respectively. To investigate the effects of PCC0208025 on the immune function in B16-F10-bearing mice, the plasma IFN-γ level was detected using mice ELISA kit. As shown in Fig 5, PCC0208025 of 30 and 60 mg/kg markedly elevated plasma IFN-γ levels compared with the control group (each treatment $P < 0.05$, $n = 6$). The work suggests that PCC0208025 exhibited anti-tumor effects in B16-F10 tumor isograft model through inhibiting Treg expansion and increasing cytotoxic activity of tumor-infiltrating CD8+ T cells by the blockade of PD-1/PD-L1 binding, which provides the pharmacological basis to develop small molecule inhibitors for PD-1/PD-L1 interactions for PCC0208025 as a lead compound.

PLoS One. 2020; 15(3): e0228339. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7098565/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.