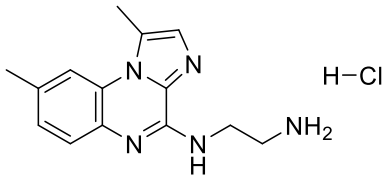
Product data sheet

MedKoo Cat#: 524432 Name: BMS-345541 HCl CAS#: 547757-23-3 (HCl) Chemical Formula: $C_{14}H_{18}ClN_5$ Exact Mass: 291.12507 Molecular Weight: 291.78	
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 345541 is a selective allosteric inhibitor of IKK (IC50 values are 0.3 and 4.0 μM for IKKβ and IKKα respectively). It attenuates LPS-induced cytokine production in vitro and blocks NFκB dependent transcription in mice. BMS 345541 also suppresses joint destruction in a mouse model of arthritis.

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	24.59	84.28
Water	29.18	100.0

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.43 mL	17.14 mL	34.27 mL
5 mM	0.69 mL	3.43 mL	6.85 mL
10 mM	0.34 mL	1.71 mL	3.43 mL
50 mM	0.07 mL	0.34 mL	0.69 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. Battula VL, Nguyen K, Sun J, Pitner MK, Yuan B, Bartholomeusz C, Hail N, Andreeff M. IKK inhibition by BMS-345541 suppresses breast tumorigenesis and metastases by targeting GD2+ cancer stem cells. Oncotarget. 2017 Jun 6;8(23):36936-36949. doi: 10.18632/oncotarget.16294. PMID: 28415808; PMCID: PMC5514883.
2. Buontempo F, Chiarini F, Bressanin D, Tabellini G, Melchionda F, Pession A, Fini M, Neri LM, McCubrey JA, Martelli AM. Activity of the selective IκB kinase inhibitor BMS-345541 against T-cell acute lymphoblastic leukemia: involvement of FOXO3a. Cell Cycle. 2012 Jul 1;11(13):2467-75. doi: 10.4161/cc.20859. Epub 2012 Jul 1. PMID: 22713244.

In vivo study

1. Zhu X, Li Q, Hu G, Wang J, Hu Q, Liu Z, Wu G, Zhong Y. BMS-345541 inhibits airway inflammation and epithelial-mesenchymal transition in airway remodeling of asthmatic mice. Int J Mol Med. 2018 Oct;42(4):1998-2008. doi: 10.3892/ijmm.2018.3762. Epub 2018 Jul 6. PMID: 30015827; PMCID: PMC6108878.
2. Yang J, Amiri KI, Burke JR, Schmid JA, Richmond A. BMS-345541 targets inhibitor of kappaB kinase and induces apoptosis in melanoma: involvement of nuclear factor kappaB and mitochondria pathways. Clin Cancer Res. 2006 Feb 1;12(3 Pt 1):950-60. doi: 10.1158/1078-0432.CCR-05-1220. PMID: 16467110; PMCID: PMC2668250.

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7. Bioactivity

Biological target:

BMS-345541 hydrochloride is a selective inhibitor of the catalytic subunits of IKK (IKK-2 IC50=0.3 μM, IKK-1 IC50=4 μM).

In vitro activity

This study found that BMS-345541 was very effective. Treatment of MDA-MB-231 cells with this agent inhibited canonical pathway-associated proteins, including pNFκB (p65), as well as non-canonical pathway-associated proteins, including RelB, in a dose-dependent manner (Figure 2A).

Reference: Oncotarget. 2017 Jun 6; 8(23): 36936–36949. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5514883/

In vivo activity

During OVA challenge, the OVA-group mice showed a variety of asthma-related symptoms, including dysphoria, shortness of breath and irregular breath rhythm, cyanosis, coughing, nose scratching and ear grasping, shrinking forelimb lift, and decreased activity. However, following treatment with BMS-345541, the asthmatic symptoms in the OVA + BMS-345541 group were significantly reduced, compared with those in the OVA and OVA + DMSO groups.

Reference: Int J Mol Med. 2018 Oct; 42(4): 1998–2008. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6108878/

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.