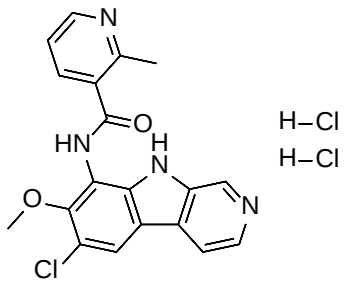
Product data sheet

MedKoo Cat#: 532254 Name: MLN120B HCl CAS: 1782573-78-7 (2HCl) Chemical Formula: $C_{19}H_{17}Cl_3N_4O_2$ Exact Mass: 366.0884 Molecular Weight: 439.721	
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:
MLN-120B is a potent and effective inhibitor of IκB kinase beta subunit (IKKβ) with IC50 value of 20 μM. MLN-120B blocks multiple myeloma cell growth in vitro and in vivo.

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	12.73	28.95
Water	2.2	5.0

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.27 mL	11.37 mL	22.74 mL
5 mM	0.45 mL	2.27 mL	4.55 mL
10 mM	0.23 mL	1.14 mL	2.27 mL
50 mM	0.05 mL	0.23 mL	0.45 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. Al-Katib A, Arnold AA, Aboukameel A, Sosin A, Smith P, Mohamed AN, Beck FW, Mohammad RM. I-kappa-kinase-2 (IKK-2) inhibition potentiates vincristine cytotoxicity in non-Hodgkin's lymphoma. Mol Cancer. 2010 Sep 1;9:228. doi: 10.1186/1476-4598-9-228. PMID: 20809973; PMCID: PMC2940845.

2. Hideshima T, Neri P, Tassone P, Yasui H, Ishitsuka K, Raje N, Chauhan D, Podar K, Mitsiades C, Dang L, Munshi N, Richardson P, Schenkein D, Anderson KC. MLN120B, a novel IkappaB kinase beta inhibitor, blocks multiple myeloma cell growth in vitro and in vivo. Clin Cancer Res. 2006 Oct 1;12(19):5887-94. doi: 10.1158/1078-0432.CCR-05-2501. PMID: 17020997.

In vivo study

1. Schopf L, Savinainen A, Anderson K, Kujawa J, DuPont M, Silva M, Siebert E, Chandra S, Morgan J, Gangurde P, Wen D, Lane J, Xu Y, Hepperle M, Harriman G, Ocain T, Jaffee B. IKKbeta inhibition protects against bone and cartilage destruction in a rat model of rheumatoid arthritis. Arthritis Rheum. 2006 Oct;54(10):3163-73. doi: 10.1002/art.22081. PMID: 17009244.

2. Nagashima K, Sasseville VG, Wen D, Bielecki A, Yang H, Simpson C, Grant E, Hepperle M, Harriman G, Jaffee B, Ocain T, Xu Y, Fraser CC. Rapid TNFR1-dependent lymphocyte depletion in vivo with a selective chemical inhibitor of IKKbeta. Blood. 2006 Jun 1;107(11):4266-73. doi: 10.1182/blood-2005-09-3852. Epub 2006 Jan 26. PMID: 16439676.

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7. Bioactivity

Biological target:

MLN120B dihydrochloride (ML120B dihydrochloride) is a potent, ATP competitive, and orally active inhibitor of IKKβ with an IC_{50} of 60 nM.

In vitro activity

MLN120B inhibits both baseline and tumor necrosis factor-alpha-induced nuclear factor-kappaB activation, associated with down-regulation of IkappaBalpha and p65 nuclear factor-kappaB phosphorylation. MLN120B triggers 25% to 90% growth inhibition in a dose-dependent fashion in multiple myeloma cell lines and significantly augments tumor necrosis factor-alpha-induced cytotoxicity in MM.1S cells. MLN120B augments growth inhibition triggered by doxorubicin and melphalan in both RPMI 8226 and IL-6-dependent INA6 cell lines.

Reference: Clin Cancer Res. 2006 Oct 1;12(19):5887-94. https://pubmed.ncbi.nlm.nih.gov/17020997/

In vivo activity

Polyarthritis was induced in rats by injection of Freund's complete adjuvant into the hind footpad. ML120B was administered orally twice daily, either prophylactically or therapeutically. Oral administration of ML120B inhibited paw swelling in a dose-dependent manner (median effective dosage 12 mg/kg twice daily) and offered significant protection against arthritis-induced weight loss as well as cartilage and bone erosion. This study was able to directly demonstrate that NF-kappaB activity in arthritic joints was reduced after ML120B administration.

Reference: Arthritis Rheum. 2006 Oct;54(10):3163-73. https://pubmed.ncbi.nlm.nih.gov/17009244/

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.