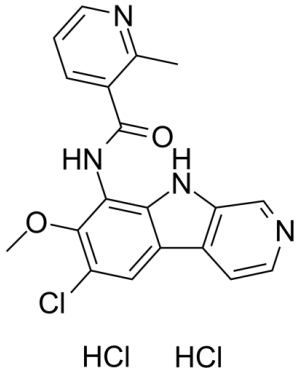
Data Sheet

Product Name:	MLN120B (dihydrochloride)
Cat. No.:	CS-0033243
CAS No.:	1782573-78-7
Molecular Formula:	$C_{19}H_{17}Cl_3N_4O_2$
Molecular Weight:	439.72
Target:	IKK
Pathway:	NF-κB
Solubility:	DMSO : 16.67 mg/mL (37.91 mM; ultrasonic and warming and adjust pH to 8 with NaOH and heat to 80°C)



BIOLOGICAL ACTIVITY:

MLN120B dihydrochloride (ML120B dihydrochloride) is a potent, ATP competitive, and orally active inhibitor of **IKKβ** with an **IC_{50}** of 60 nM. MLN120B inhibits multiple myeloma cell growth in vitro and in vivo and also can be used for the research of rheumatoid arthritis[1][2]. **In Vitro:** MLB120B (0-20 μM; 90 minutes) inhibits phosphorylation and degradation of IκB in RPMI 8226 and INA6 cells; however, no significant inhibition is observed in MM.1S cells[1].

MLB120B (1.25-20 μM; 90 minutes) completely abrogates TNF-a-induced phosphorylation and degradation of IκB in a dosedependent fashion. Phosphorylation of p65 NF-κB induced by TNF-a is also blocked by MLN120B[1].

MLN120B inhibits proliferation of multiple myeloma cell lines. MM.1S, MM.1R, RPMI 8226, RPMI-LR5, RPMI-Dox40, U266, and INA6 cells. Five percent to fifty percent and 18% to 70% inhibition in proliferation is observed at doses >20 uM and [^{3}H]thymidine uptake, respectively[1].

MLN120B (1.25-40 μM; 72 hours) almost completely blocks stimulation of MM.1S, U266, and INA6 cell growth, as well as IL-6 secretion from BMSCs, induced by multiple myeloma cell adherence to BMSCs[1].

MLN120B shows an inhibitory effect on LPS induced NF-κB activation in RAW267.4 cells. The IC_{50} values of MLN120B is 1.4 μM, 14.8 μM or 27.3 μM for NF-κB2-luc2, IL8-luc2 or TNF-AIP3-luc2 reporter transfected cells, respectively[3].

In Vivo: MLN120B (oral administration; 50 mg/kg; twice daily; 3 weeks) induces a reduction of shuIL-6R, marker of tumor growth, marker of tumor growth. It also leads to a rend toward prolonged survival in animals treated versus control[1].

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References:

[1]. Hideshima T, et all. 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.

[2]. Schopf L, et al. IKKbeta inhibition protects against bone and cartilage destruction in a rat model of rheumatoid arthritis. Arthritis Rheum. 2006 Oct;54(10):3163-73.

[3]. Ansaldi D, et al. Imaging pulmonary NF-kappaB activation and therapeutic effects of MLN120B and TDZD-8. PLoS One. 2011;6(9):e25093.

[4]. [3].Nagashima K, et al. Rapid TNFR1-dependent lymphocyte depletion in vivo with a selective chemical inhibitor of IKKbeta. Blood. 2006 Jun 1;107(11):4266-73.

CAIndexNames:

3-Pyridinecarboxamide, N-(6-chloro-7-methoxy-9H-pyrido[3,4-b]indol-8-yl)-2-methyl-, hydrochloride (1:2)

SMILES:

ClC1=C(C(NC(C2=CC=CN=C2C)=O)=C3C(C4=C(N3)C=NC=C4)=C1)OC.Cl.Cl

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