

Product Name: ML 120B dihydrochloride

Catalog No.: 4899

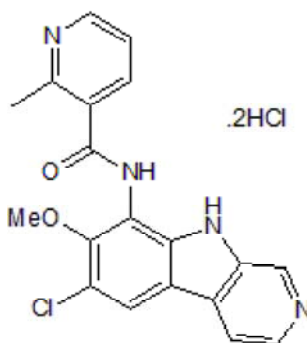
Batch No.: 1

CAS Number: 1782573-78-7

IUPAC Name: *N*-(6-Chloro-7-methoxy-9*H*-pyrido[3,4-*b*]indol-8-yl)-2-methyl-3-pyridinecarboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₅ClN₄O₂·2HCl·¾H₂O
Batch Molecular Weight: 453.23
Physical Appearance: Yellow solid
Solubility: DMSO to 20 mM
 water to 5 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.1 (Chloroform:Methanol [9:1])
HPLC: Shows 98% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.35	4.11	12.36
Found	50.28	4.26	12.23

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Novel, ATP-competitive IKK2-selective inhibitor (IC_{50} = 60 nM at 50 μ M ATP). Exhibits no inhibition at IKK1 (EC_{50} >100 μ M), IKK ϵ (EC_{50} >100 μ M) or a panel of 28 other kinases (EC_{50} >50 μ M). Exhibits antitumor activity in lymphoma-bearing SCID mice. Demonstrates synergistic cytotoxic effects with vincristine (Cat. No. 1257).

Physical and Chemical Properties:

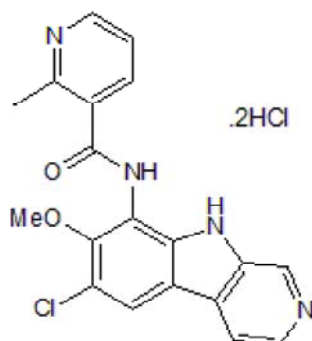
Batch Molecular Formula: C₁₉H₁₅ClN₄O₂·2HCl· $\frac{3}{4}$ H₂O

Batch Molecular Weight: 453.23

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM

water to 5 mM with gentle warming

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Al-Katib *et al* (2010) I-kappa-kinase-2 (IKK-2) inhibition potentiates vincristine cytotoxicity in non-Hodgkin's lymphoma. *Mol.Cancer* **9** 1476. PMID: 20809973.

Catley *et al* (2006) Validation of the anti-inflammatory properties of small-molecule I kappaB Kinase (IKK)-2 inhibitors by comparison with adenoviral-mediated delivery of dominant-negative IKK1 and IKK2 in human airways smooth muscle. *Mol.Pharmacol.* **70** 697. PMID: 16687566.

Nagashima *et al* (2006) Rapid TNFR1-dependent lymphocyte depletion in vivo with a selective chemical inhibitor of IKKbeta. *Blood* **107** 4266. PMID: 16439676.

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