

Product Name: MRT 67307 dihydrochloride

Catalog No.: 5134

Batch No.: 1

IUPAC Name: *N*-[3-[[[5-Cyclopropyl-2-[[3-(4-morpholinylmethyl)phenyl]amino]-4-pyrimidinyl]amino]propyl]cyclobutanecarboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₃₆N₆O₂·2HCl·½H₂O

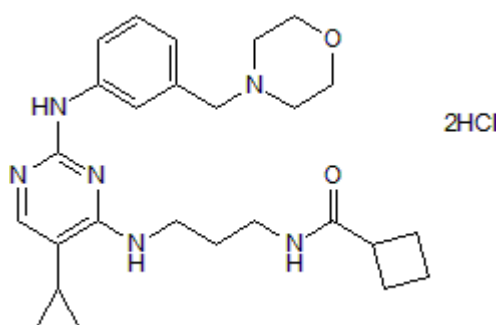
Batch Molecular Weight: 546.53

Physical Appearance: Beige solid

Solubility: water to 20 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.12 (Chloroform:Methanol [9:1])

HPLC: Shows >98.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.14	7.19	15.38
Found	57.14	7.58	15.12

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

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Description:

Salt inducible kinase (SIK) inhibitor (IC₅₀ values are 67, 250 and 430 nM for SIK2, SIK1 and SIK3 respectively). Also inhibits TBK1, MARK1-4, IKKε and NUA1 (IC₅₀ values are 19, 27-52, 160 and 230 nM respectively). Has no effect on IKKα or IKKβ. Induces IL-10 secretion and inhibits TNF-α and IL-6 secretion in bacterial LPS-stimulated macrophages. Also enhances IL-1-induced activation of NFκB-dependent gene transcription in mouse embryonic fibroblast (MEF) cells.

Physical and Chemical Properties:

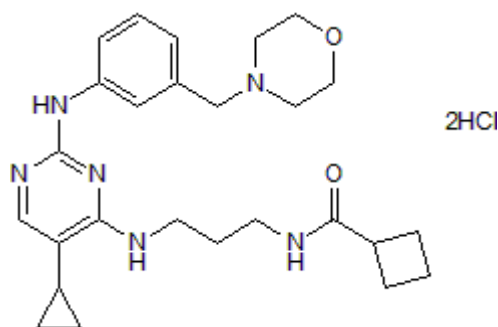
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Batch Molecular Weight: 546.53

Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 20 mM

DMSO to 100 mM

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:

Clark et al (2011) Novel cross-talk within the IKK family controls innate immunity. *Biochem.J.* **434** 93. PMID: 21138416.

Smith et al (2011) The role of TBK1 and IKKε in the expression and activation of Pellino 1. *Biochem.J.* **434** 537. PMID: 21204785.

Clark et al (2012) Phosphorylation of CRTC3 by the salt-inducible kinases controls the interconversion of classically activated and regulatory macrophages. *Proc.Natl.Acad.Sci.U.S.A.* **109** 16986. PMID: 23033494.

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