

Product Name: MRT 68921 dihydrochloride

Catalog No.: 5780

Batch No.: 1

CAS Number: 2080306-21-2

IUPAC Name: *N*-[3-[[[5-Cyclopropyl-2-[(1,2,3,4-tetrahydro-2-methyl-6-isoquinolinyl)amino]-4-pyrimidinyl]amino]propyl]cyclobutanecarboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₃₄N₆O·2HCl·¼H₂O

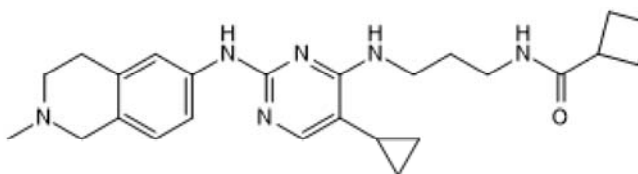
Batch Molecular Weight: 512

Physical Appearance: White solid

Solubility: water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2HCl

2. ANALYTICAL DATA

TLC: R_f = 0.32 (5% (7M ammonia in MeOH)/DCM)

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.65	7.19	16.41
Found	58.68	7.17	16.4

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

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Description:

MRT 68921 dihydrochloride is a potent ULK inhibitor (IC₅₀ values are 1.1 and 2.9 nM for ULK2 and ULK1, respectively). Inhibits autophagy in mouse embryonic fibroblasts.

Physical and Chemical Properties:

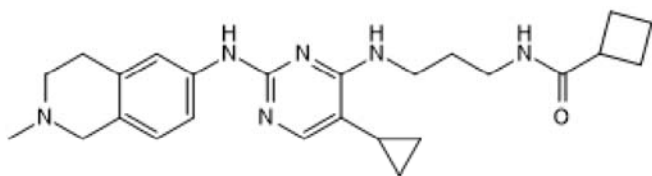
Batch Molecular Formula: C₂₅H₃₄N₆O.2HCl.¼H₂O

Batch Molecular Weight: 512

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



2HCl

Storage: Desiccate at RT

Solubility & Usage Info:

water 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:

Petherick et al (2015) Pharmacological inhibition of ULK1 kinase blocks mammalian target of rapamycin (mTOR)-dependent autophagy. *J.Biol.Chem.* **290** 11376. PMID: 25833948.

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