Print Date: Mar 9th 2021

Certificate of Analysis

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Product Name: **MRT 68601 hydrochloride** **Catalog No.: 5067** **Batch No.: 1**

CAS Number: 1962928-25-1

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{34}N_6O_2.HCl.H_2O$

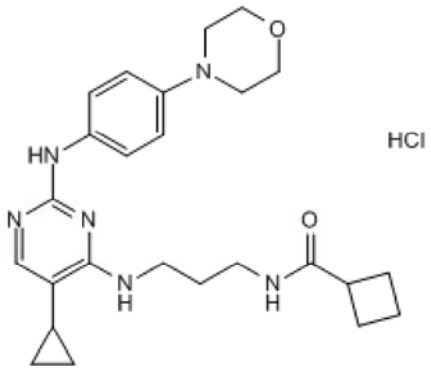
Batch Molecular Weight: 505.06

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.18 (Dichloromethane:Methanol [9:1])

HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.45	7.38	16.64
Found	59.24	7.18	16.43

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Product Information

Product Name: **MRT 68601 hydrochloride** **Catalog No.: 5067** **Batch No.: 1**

CAS Number: 1962928-25-1

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

Description:

Potent TBK1 (TANK-binding kinase-1) inhibitor (IC_{50} = 6 nM). Inhibits the formation of autophagosomes in lung cancer cells.

Physical and Chemical Properties:

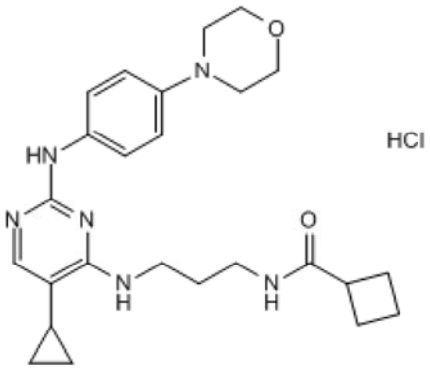
Batch Molecular Formula: $C_{25}H_{34}N_6O_2.HCl.H_2O$

Batch Molecular Weight: 505.06

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at RT. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM
ethanol 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:

McIver *et al* (2012) Synthesis and structure-activity relationships of a novel series of pyrimidines as potent inhibitors of TBK1/IKKe kinases. Bioorg.Med.Chem.Lett. ***22*** 7169. PMID: 23099093.

Newman *et al* (2012) TBK1 kinase addiction in lung cancer cells is mediated via autophagy of Tax1bp1/Ndp52 and non-canonical NF-κB signalling. PLoS ONE ***7*** e50672. PMID: 23209807.