

Product Name: TC-S 7001

Catalog No.: 4961

Batch No.: 1

CAS Number: 867017-68-3

IUPAC Name: 6-Chloro-*N*⁴-[3,5-difluoro-4-[(3-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-4-yl)oxy]phenyl]-2,4-pyrimidinediamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₃ClF₂N₆O.1½H₂O

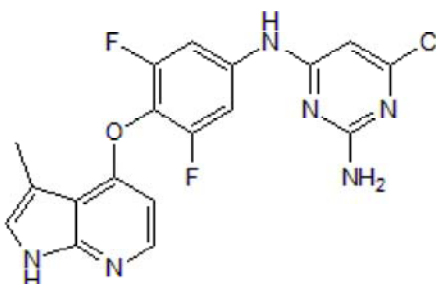
Batch Molecular Weight: 429.81

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.3	3.75	19.55
Found	50.31	3.45	19.38

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

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Description:

TC-S 7001 (also known as BAY-549) is a potent and highly selective ROCK inhibitor (IC₅₀ values are 0.6 and 1.1 nM for human ROCK1 and ROCK2, respectively), which exhibits >200-fold selectivity over TRK and FLT3 receptors, and >900-fold selectivity over a panel of other kinases and cardiovascular relevant enzymes and receptors. TC-S 7001 reduces blood pressure in normotensive and hypertensive rats, and is orally active.

Physical and Chemical Properties:

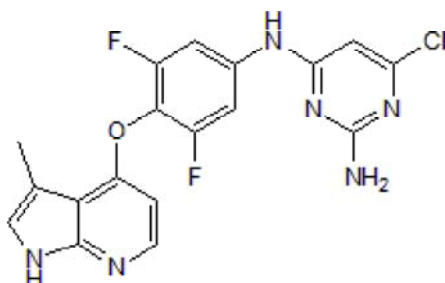
Batch Molecular Formula: C₁₈H₁₃ClF₂N₆O.1½H₂O

Batch Molecular Weight: 429.81

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Dahal et al (2010) Therapeutic efficacy of azaindole-1 in experimental pulmonary hypertension. *Eur.Resp.J.* **36** 808. PMID: 20530035.

Kast et al (2007) Cardiovascular effects of a novel potent and highly selective azaindole-based inhibitor of Rho-kinase. *Br.J.Pharmacol.* **152** 1070. PMID: 17934515.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 100 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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.

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