

Product Name: RKI 1447 dihydrochloride

Catalog No.: 5061

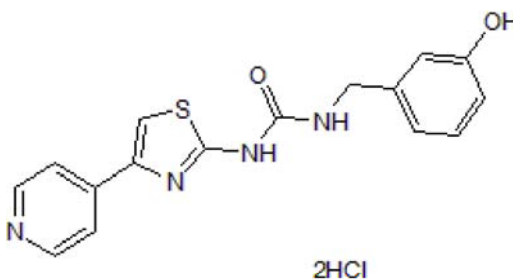
Batch No.: 1

CAS Number: 1782109-09-4

IUPAC Name: *N*-[(3-Hydroxyphenyl)methyl]-*N'*-[4-(4-pyridinyl)-2-thiazolyl]urea dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₄N₄O₂S.2HCl.2H₂O
Batch Molecular Weight: 435.32
Physical Appearance: Beige solid
Solubility: water to 10 mM with gentle warming
DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Dichloromethane:Methanol: Aqueous Ammonia [8:9:1:0])
HPLC: Shows 99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	44.15	4.63	12.87
Found	44.45	4.78	12.88

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

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Description:

Potent and selective ROCK inhibitor (IC₅₀ values are 6.2 and 14.5 nM for ROCK2 and ROCK1 respectively); suppresses phosphorylation of ROCK substrates MLC-2 and MYPT-1 in human cancer cells, but has no effect on the phosphorylation levels of Akt, MEK, and S6 kinase. Displays anti-invasive and antitumor activities in breast cancer cells.

Physical and Chemical Properties:

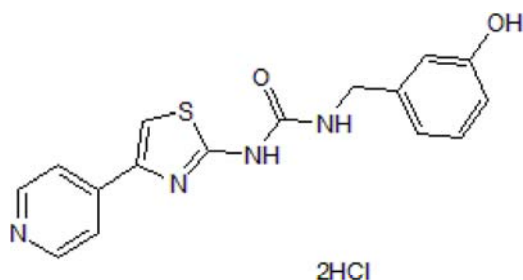
Batch Molecular Formula: C₁₆H₁₄N₄O₂S.2HCl.2H₂O

Batch Molecular Weight: 435.32

Physical Appearance: Beige solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 10 mM with gentle warming
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:

Pireddu et al (2013) Pyridylthiazole-based ureas as inhibitors of Rho associated protein kinases (ROCK1 and 2) *Med.Chem.Comm.* **3** 699. PMID: 23275831.

Patel et al (2012) RKI-1447 is a potent inhibitor of the Rho-associated ROCK kinases with anti-invasive and antitumor activities in breast cancer. *Cancer Res.* **72** 5025. PMID: 22846914.

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