

IUPAC Name:

Certificate of Analysis

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Product Name: RU-SKI 43 hydrochloride

Catalog No.: 4886 Batch No.: 1 2-((2-Methylbutyl)amino)-1-(4-((3-methylphenoxy)methyl-6,7-dihydrothieno[3,2-c]pyridin-5(4H)-yl)ethanone

hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{22}H_{30}N_2O_2S.HCI.4H_2O$ **Batch Molecular Formula:**

Batch Molecular Weight: 427.51 White solid **Physical Appearance:**

DMSO to 100 mM Solubility: Store at +4°C Storage:

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure **Mass Spectrum:** Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 61.81 7.43 6.55 Found 61.84 7.24 6.47





Product Information

Print Date: May 15th 2014

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hydrochloride

Description:

Hedgehog acyltransferase (Hhat) inhibitor ($IC_{50} = 850$ nM). Inhibits Sonic Hedgehog N (ShhN) palmitoylation in vitro. Has no effect on porcupine-induced fatty acid acylation of Wnt39a. Attenuates pancreatic cancer cell proliferation. Cell permeable.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{22}H_{30}N_2O_2S.HCI.\frac{1}{4}H_2O$

Batch Molecular Weight: 427.51 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

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:

Petrova et al (2013) Inhibitors of Hedgehog acyltransferase block Sonic Hedgehog signaling. Nat.Chem.Biol. 9 247. PMID: 23416332.

Petrova et al (2014) Hedgehog acyltransferase as a target in pancreatic ductal adenocarcinoma. Oncogene. PMID: 24469057.

