

Certificate of Analysis

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Product Name: Y 39983 dihydrochloride

Catalog No.: 3846

Batch No.: 1

CAS Number: 203911-26-6

IUPAC Name: 4-[(1*R*)-1-Aminoethyl]-*N*-1*H*-pyrrolo[2,3-*b*]pyridin-4-ylbenzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₆N₄O.2HCl.1¾H₂O

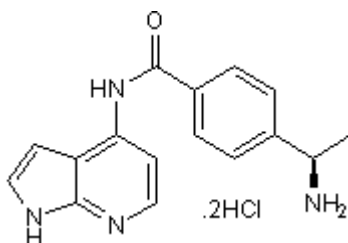
Batch Molecular Weight: 384.77

Physical Appearance: Off-white solid

Solubility: water to 100 mM
DMSO to 100 mM
ethanol to 5 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +5.4 (Concentration = 1, Solvent = Methanol)

Microanalysis:

Carbon Hydrogen Nitrogen

| | | | |
|-------------|-------|------|-------|
| Theoretical | 49.94 | 5.63 | 14.56 |
| Found | 49.95 | 5.52 | 14.46 |

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

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Description:

Selective Rho-kinase inhibitor (IC₅₀ values are 0.0036, 0.42 and 0.81 μM for ROCK, PKC and CaMKII respectively). Promotes neurite regeneration in vitro and induces axonal regeneration in vivo. Derived from Y-27632 (Cat. No. 1254).

Physical and Chemical Properties:

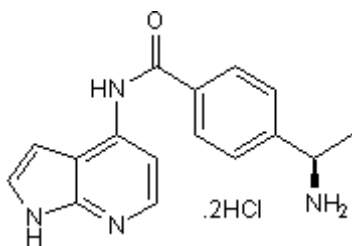
Batch Molecular Formula: C₁₆H₁₆N₄O.2HCl.1¾H₂O

Batch Molecular Weight: 384.77

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM
ethanol to 5 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:

Sagawa et al (2007) A novel ROCK inhibitor, Y-39983, promotes regeneration of crushed axons of retinal ganglion cells into the optic nerve of adult cats. *Exp.Neurol.* **205** 230. PMID: 17359977.

Tokushige et al (2007) Effects of topical administratino of Y-39983, a selective Rho-associated protein kinase inhibitor, on ocular tissues in rabbits and monkeys. *Invest.Ophthalmol.Vis.Sci.* **48** 3216.

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