

Certificate of Analysis

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Product Name: AS 1892802

Catalog No.: 4927

Batch No.: 1

CAS Number: 928320-12-1

IUPAC Name: *N*-[(1*S*)-2-Hydroxy-1-phenylethyl]-*N'*-[4-(4-pyridinyl)phenyl]-urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₉N₃O₂·¼H₂O

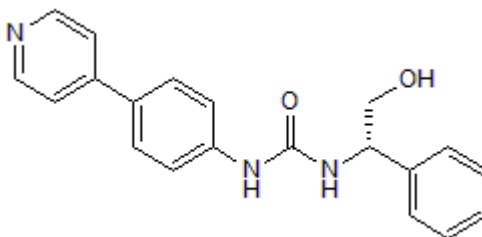
Batch Molecular Weight: 337.88

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.45 (Chloroform:Methanol [9:1])

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +85.8 (Concentration = 0.68, Solvent = Methanol)

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 71.09 5.82 12.44

Found 71.38 5.71 12.54

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

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Description:

Potent, ATP-competitive ROCK inhibitor (IC₅₀ values are 52, 57 and 122 nM for human ROCK2, rat ROCK2 and human ROCK1 respectively by ELISA); also inhibits PKAC- α and PRKX (IC₅₀ values are 200 and 325 nM respectively). Exhibits analgesic effects in rat models of inflammatory (AIA) and noninflammatory (MIA) arthritic pain. Orally bioavailable.

Physical and Chemical Properties:

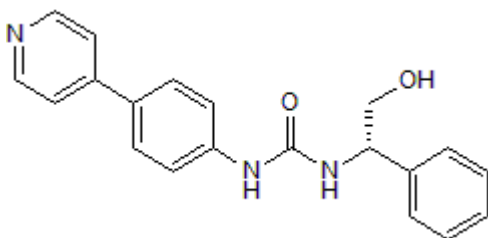
Batch Molecular Formula: C₂₀H₁₉N₃O₂·¼H₂O

Batch Molecular Weight: 337.88

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Yoshimi *et al* (2010) Antinociceptive effects of AS1892802, a novel Rho kinase inhibitor, in rat models of inflammatory and noninflammatory arthritis. *J.Pharmacol.Exp.Ther.* **334** 955. PMID: 20534789.

Li *et al* (2012) Fragment-based and structure-guided discovery and optimization of Rho kinase inhibitors. *J.Med.Chem.* **55** 2474. PMID: 22272748.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 25 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.

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