

Product Name: H 1152 dihydrochloride

Catalog No.: 2414

Batch No.: 4

CAS Number: 871543-07-6

IUPAC Name: (S)-(+)-2-Methyl-1-[(4-methyl-5-isoquinolinyl)sulfonyl]-hexahydro-1H-1,4-diazepine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₂₁N₃O₂S.2HCl

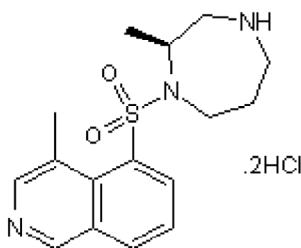
Batch Molecular Weight: 392.34

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 50 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.38 (Chloroform:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +18.8 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.98	5.91	10.71
Found	49.09	6.05	10.41

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Description:

H 1152 dihydrochloride is a rho-kinase (ROCK) inhibitor that displays high selectivity over other protein kinases (IC₅₀ values are 0.012, 0.180, 0.360, 0.745, 3.03, 5.68 and 28.3 μM for ROCKII, CAMKII, PKG, Aurora A, PKA, PKC and MLCK respectively). Inhibits sulprostone-induced contractions in guinea pig aorta (IC₅₀ = 190 nM) and displays proerectile effects in rats. Glycyl Derivative also available.

Physical and Chemical Properties:

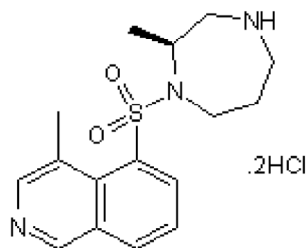
Batch Molecular Formula: C₁₆H₂₁N₃O₂S.2HCl

Batch Molecular Weight: 392.34

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Tamura et al (2005) Development of specific Rho-kinase inhibitors and their clinical application. *Biochim.Biophys.Acta* **1754** 245. PMID: 16213195.

Teixeira et al (2005) Proerectile effects of the rho-kinase inhibitor (S)-(+)-2-methyl-1-[(4-methyl-5-isoquinolinyl)sulfonyl]homopiperazine (H-1152) in the rat penis. *J.Pharmacol.Exp.Ther.* **315** 155. PMID: 15976017.

Shum et al (2003) Involvement of Rho-kinase in contraction of guinea-pig aorta induced by prostanoid EP₃ receptor agonist. *Br.J.Pharmacol.* **139** 1449. PMID: 12922932.

Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 100 mM

DMSO to 50 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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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