TOCRIS
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Print Date: Jan 11th 2016

Certificate of Analysis

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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-1*H*-1,4-diazepine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{21}N_3O_2S.2HCl$

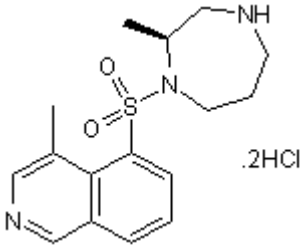
Batch Molecular Weight: 392.34

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

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +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:

Rho-kinase (ROCK) inhibitor that displays high selectivity over other protein kinases (IC_{50} 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 (IC_{50} = 190 nM) and displays proerectile effects in rats. Glycyl derivative available (Cat. No. 2485).

Physical and Chemical Properties:

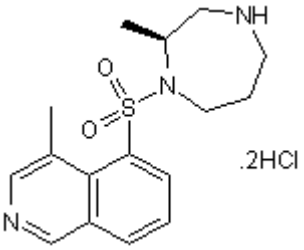
Batch Molecular Formula: $C_{16}H_{21}N_3O_2S.2HCl$

Batch Molecular Weight: 392.34

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 100 mM
DMSO to 50 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:

Shum *et al* (2003) Involvement of Rho-kinase in contraction of guinea-pig aorta induced by prostanoid EP_3 receptor agonist. Br.J.Pharmacol. ***139*** 1449. PMID: 12922932.

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.

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