

Product Name: SR 3677 dihydrochloride

Catalog No.: 3667

Batch No.: 2

CAS Number: 1781628-88-3

IUPAC Name: *N*-[2-[2-(Dimethylamino)ethoxy]-4-(1*H*-pyrazol-4-yl)phenyl]-2,3-dihydro-1,4-benzodioxin-2-carboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₄N₄O₄·2HCl·½H₂O

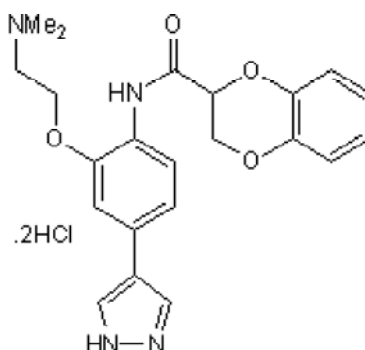
Batch Molecular Weight: 490.38

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.88	5.55	11.43
Found	53.9	5.62	11.45

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

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Description:

Potent and selective Rho-kinase inhibitor (IC₅₀ values are 3 and 56 nM for ROCK-II and ROCK-I respectively).

Physical and Chemical Properties:

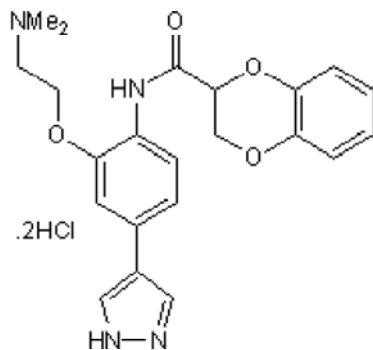
Batch Molecular Formula: C₂₂H₂₄N₄O₄·2HCl·½H₂O

Batch Molecular Weight: 490.38

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM

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:

Feng *et al* (2008) Discovery of substituted 4-(pyrazol-4-yl)-phenylbenzodioxane-2-carboxamides as potent and highly selective Rho kinase (ROCK-II) inhibitors. *J.Med.Chem.* **51** 6642. PMID: 18834107.

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